

Towards Automated Determination of USERMAT for the Nonlinear Constitutive Behavior of Composites

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Abstract

Over the last 30 years NRL's Composite Materials and Structures (CMS) group has been developing a data driven system identification inverse approach for characterizing the constitutive behavior of polymer matrix composites (PMCs). The core concept in this approach has been the experimental identification of a dissipated energy density (DED) function. This is achieved through establishing a non-linear optimization scheme for determining the free coefficients of the sum of the basis functions that are used to construct the DED function and is based on the energy balance of the specimen under test. The method used was based on using massive amounts of experimental data that would be produced by exposing PMC specimens to multidimensional loading paths with the help of custom made multi-axial computer-controlled testing machines. The analytical and numerical implementation that has been followed up to now has been developed within various custom environments and this has been one of the main stumbling blocks in transferring this technology to end users in the design and material communities.

Recent advances in finite element techniques and design optimization integration technologies along with the parallel hardware and software evolution have directed the CMS group to turn its attention to utilizing "of the shelf" technology of achieving the same goals. Thus, the "Z-mat" and "Z-Optim" packages from Northwest Numerics, Inc., have been utilized to extract the non-linear constitutive response from the available experimental data in an integrated and automated manner and in conjunction with the ANSYS/Mechanical infrastructure. The automation lies on the fact that the process automatically generates the code of a "USERMAT" subroutine that it can be subsequently used with any geometry and loading specification definable within the limits of ANSYS' non-linear element library. The geometry of the single notched specimen of NRL's In Plane has been used for developing and verifying the process.

Introduction

For the past thirty years NRL's Composite Materials and Structures group has been systematically utilizing computational technology to automate the engineering research process. One of the most dominant of these efforts was the task of automated experimentation of composite material specimens in order to identify their (constitutive) behavior in multidimensional loading spaces. Design, construction and utilization of custom multi-degree of freedom loading machines along with an automated inverse approach implementation allowed achieving the goal of automated characterization of composites [1-5].

One of the hardest lessons to learn was that having a technology that is successful in terms of solving various problems in the area of composite material design qualification and certification, does not necessarily mean that this technology is also successful in helping domain experts to solve their problems. If this technology cannot be transferred from the producer into the consumers' activity space in a way that allows them to extract value out of it, then it does not succeed in being a useful technology. The problem was that the traditional approaches such as publications, workshops, tutorials etc. could not succeed as media for technology transfer. One of the criticisms we heard many times was that we were using many "custom" solutions and our customers were not willing to invest in "special resources expenditures" just to use something that appear very complex. Since complexity is not always a property of the tool one uses, but also is a measure of the user's own knowledge about the domain of expertise within which the tool is

definable, we focused on attempting to create a solution to the technology transfer problem that is based -as much as possible- to already existing tools where users had already invested their learning dues and they had also acquired own specialized experience and expertise.

Since the experimental part of our technology is not transferable at this time, we felt that we should seek for an implementation of our software technology focusing in third party resources in three main areas: public domain software, innovative commercial software, and industrial strength commercial software. Public software allows customers to use ubiquitous technology with no monetary expenses. Innovative commercial software allows customers to rely on the provider's technical support and training while he takes advantage of unique technological innovation at the interface between the bleeding edge of research and the freedom of usage edge of commerce. Industrial strength commercial software, allows users to exploit an existing resource with many years of knowledge as well as user and development experience.

This paper is reporting our first attempt to achieve this goal of implementing our technology by exploiting as many of the benefits reported for each one of the available software categories.

ANSYS Problem Definition Language (APDL) [06] provides an immense flexibility for modeling and analysis of structural models by using ANSYS [07], and this was the reason we had selected it as our "industrial strength commercial" representative. Coincidentally, many vertical industries in need of Finite Element Modeling (FEM) and Analysis (FEA) have already invested into ANSYS and this makes our choice an appropriate application for our purposes.

The Z-set suite of tools and especially the Z-mat package by Northwest Numerics Inc. [08-10], are the results of a cooperative effort between the company and the French organizations Transvator, Ecole des Mines, Materials Research Centre, ONERA, and INSA de Rouen. It represents our second choice for this effort and it falls in the category of innovative commercial software at the bleeding interface between research and commerce. These tools were selected because of two unique features:

- the immense flexibility in allowing users to define custom material behavior for their FEA needs, in a dynamic and polymorphic manner [10],
- the extremely unique implementation of optimization technology that allows utilization of experimental data for the determination of constitutive models.

These features helped us enormously in reducing the custom code development and they allowed us to achieve all of our goals, but especially the one about not using custom code.

The only resource that the new scheme still utilizes that was present during our past implementations is our database content of test data.

The present paper contains the a description of the data acquisition methodology along with a quick review of the old way of characterizing composite behavior via the use of dissipated energy density (DED). What follows is a description of the Z-set, Z-mat based process that we are developing in place of the original. We end with some examples of its usage and concluding remarks.

Multidimensional Characterization of PMCs (Original Approach)

In order to characterize the constitutive response of a PMC system, NRL has developed a system identification approach utilizing custom made testing machines that exposes material specimens to discrete loading paths spanning the loading space of the specimen structure. Two characteristic examples of such machines are the In Plane Loader System (IPLS) and the Six Degree of freedom Loader System (6DLS) shown in figure 1. Details about these machines and the associated automated processes are given extensively in [1-5].

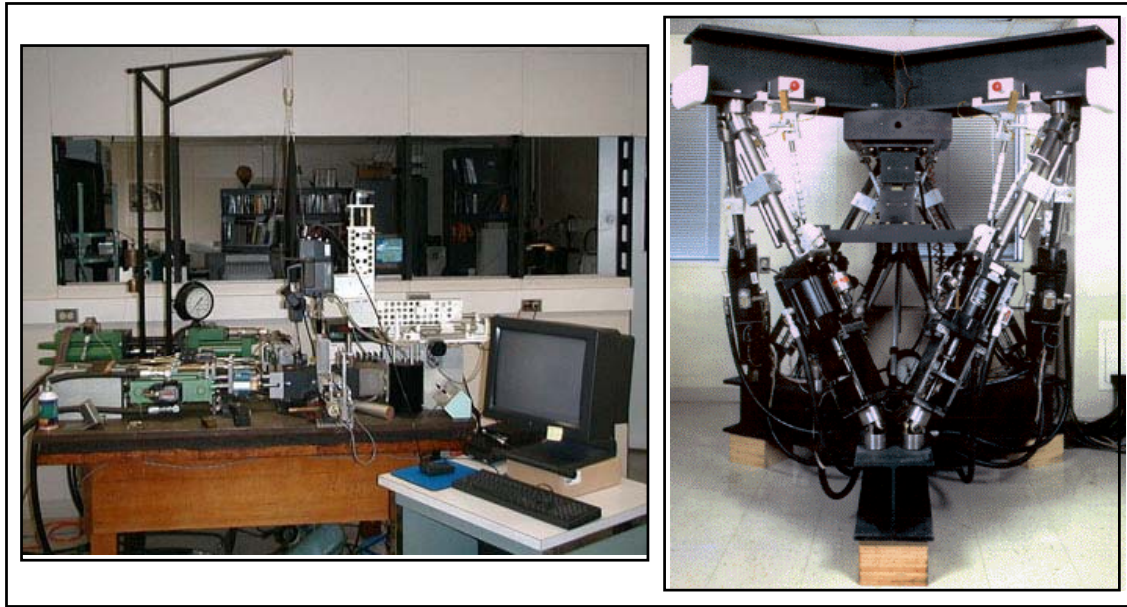


Figure 1 - Views of IPLS (left) and the 6DLS (right).

Specimen Considerations

Composite materials associated with various applications range through a wide variety of constituent materials. Each different combination of matrix, fiber, fiber coating (for matrix-fiber interphase), layup angle, stacking sequence, etc. corresponds to a different material. The approach discussed here is specifically tailored to PMCs. Approximately 100 material systems with fibers ranging from Kevlar to IM7 graphite and several thermoset resins and thermoplastic organic polymers have been tested and characterized with the approach discussed here. A partial list of all the materials tested up to now can be found in [2].

The specimen geometry was designed to satisfy the following requirements:

- The characteristic dimensions should be large enough relative to fiber diameter and lamina thickness to ensure that the material could be analyzed as either a single mechanically equivalent homogeneous anisotropic monolithic material, or a collection of layers of varying orientations of such materials.
- The overall specimen size should be small enough to keep material costs at a manageable level.
- Strain riser(s) (such as notches, holes etc.) should be present to guarantee that high strain regions occur well away from all specimen boundaries.

Experimental Procedure

The objective of the IPLS is to control the rigid body motion of the boundary of the specimen that is held by the movable grip and at the same time measure the boundary displacements and tractions. Because the actuators of the IPLS are constrained to move in a plane parallel to the specimen, the resulting motion involves only three degrees of freedom relative to any frame of reference on that plane. As it can be seen in figure 2 the grip motion can be resolved into three basic components: sliding (shearing) u_0 , opening/closing u_1 , and in-plane rotation u_2 . Specified combinations of actuator displacements, therefore, map into particular combinations of these three basic motions.

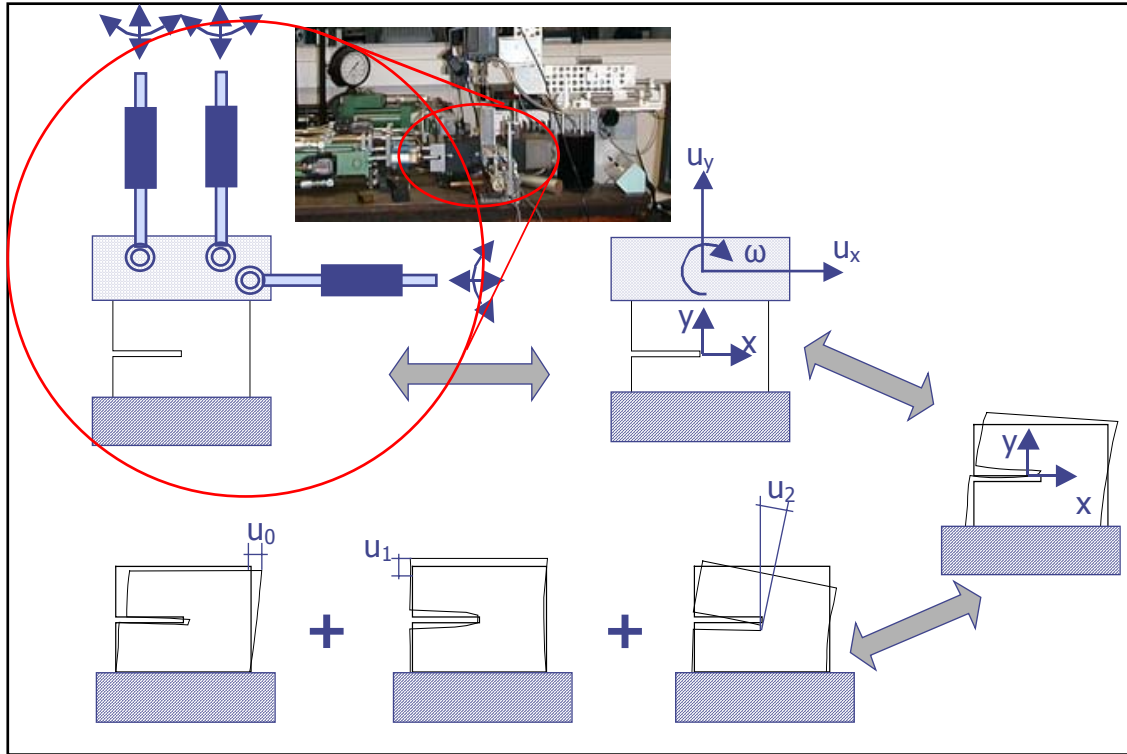


Figure 2 - Loading Modes of the In Plane Loader

In order to visualize the loading space it is advantageous to think in terms of a three dimensional displacement space with coordinates (u_0, u_1, u_2) . The issue then is how to select a representative family of paths that cover the space and how to sample along each path. It was decided to cover the boundary displacement space with a set of 15 uniformly distributed radial loading paths as indicated in Fig. 3. Note that because of geometry and material symmetry about the axis along the notch(es), only the half space corresponding to positive sliding displacement ($u_0 > 0$) need be considered. The required set of observation points is generated by sampling boundary displacement and force data along each path. A particular test in which the actuator motions are continuously varied corresponds to a specific path in this space. Only 15 specimens are required, and 50 observations per loading path are obtained from a single specimen.

The locus of the end points of all loading paths for the same increment is a sphere as shown in figure 3, where two arbitrary loading paths at three arbitrary increments are presented as an example along with the two basis case loading paths of pure shearing, and opening.

The traditional NRL methodology for PMC characterization uses the Dissipated Energy Density Function (DEDF) as a storage mechanism for their constitutive behavior. The spatial distributions of dissipated energy density after the DEDF has been determined via the process described below, are shown also in Fig. 3 at three specific points on its one of the chosen loading paths for the double notched specimen used for the 6DLS, for a particular PMC system.

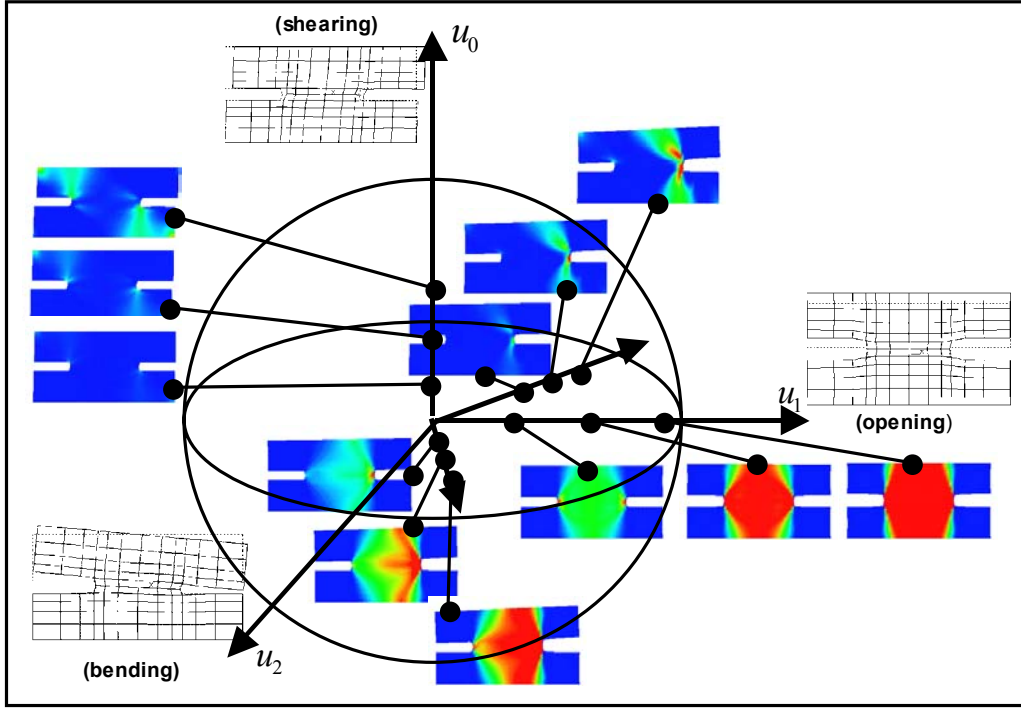


Figure 3 - In plane loading space and associated loading paths along with post computed distributions of dissipated energy density of specimens at corresponding points of selected loading paths.

The set of activities associated with the traditional methodology of determining the DEDF along with their interrelationship are shown in the Universal Modeling Language (UML) [11] activity diagram of figure 4.

The process of computing the total dissipated energy is based on the boundary displacements and tractions that are measured at each increment imposed by the IPLS along each loading path. More details are presented elsewhere [2-5]. One specimen per loading path is used initially and the procedure is then repeated for a total of two specimens per loading path.

The DEDF is constructed as a sum of basis functions χ_i that depend only on the local strain state $\tilde{\mathcal{E}}$ of the material in the structure, and are weighted by coefficients c_i that depend only on the material:

$$\phi(\tilde{\mathcal{E}}, m) = \phi(\tilde{\mathcal{E}}, \tilde{c}) = c_1(m)\chi_1(\tilde{\mathcal{E}}) + c_2(m)\chi_2(\tilde{\mathcal{E}}) + \dots + c_n(m)\chi_n(\tilde{\mathcal{E}}) \quad (1)$$

This particular form for ϕ , accomplishes a full decomposition of the effects of the geometry from those of the material by forcing it to be only a function of the strain state. It also, accomplishes scale independence within the domain of application of the continuum hypothesis.

Determination of the dissipated energy density function can be accomplished by employing a desirable vector space defining the polynomials representing the basis functions, and subsequently determine the coefficients c_i . This is accomplished by considering the energy balance equation,

$$\int_0^{u_r} t_u q_v dq^v - \frac{1}{2} t_s u_t u^v = \int_{\partial V} \phi(\epsilon_i(x_j)) dx_j \quad (2)$$

The left hand side represents the dissipated energy lost in the structure as the difference between the total energy imparted by the testing machine to the specimen, minus the recoverable energy. Where t and u are

used to name the components of the boundary tractions and displacements respectively. This side of the equation is determined at the end of the left path through the red activities of figure 4.

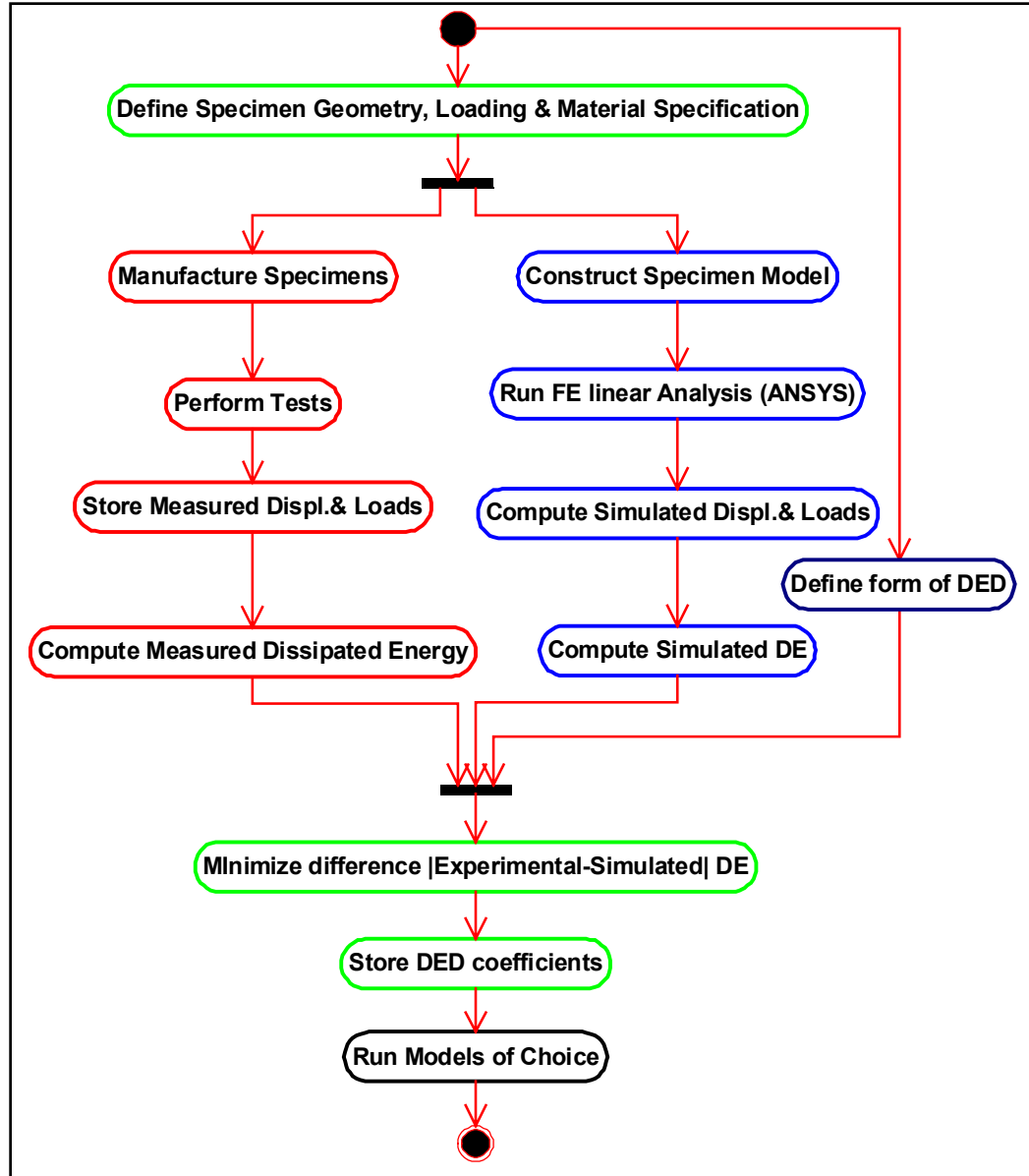


Figure 4 - UML activity diagram of the DED determination process.

The right hand side of Eq. (3) represent the dissipated energy list in the structure as the integral over the volume of the specimen of the dissipated energy density function. This side of the equation is determined at the end of the right path through the red activities of figure 4.

The discrete form of this equation -resulting from consideration of the total energy as the sum of energies for each finite element of the model for the specimen-, can be written for as many times as needed in order to define an overdetermined system of linear equations with c_i as unknowns. Since this system is overdetermined, and since we have to consider the monotonicity and positive definiteness of ϕ , the problem can be considered to be a global optimization problem with inequality constraints. Various

algorithms are available to use for solving this problem. We have been using random hill climb with reversal algorithm as it has been captured in the ACM TOMS library algorithm 587 [12]. When the c_i unknowns are determined they are saved in a database for further use in simulating the behavior of the material in geometries of the user's choice.

The DED concept has been applied to many applications that require factual determination of PMC behavior characterization including applications for establishing a metric for distributed health assessment in smart structures [13-15].

Automated Multidimensional Characterization of PMCs (Current Approach).

To follow the decision of utilizing non custom tools and in order to embed the non-linear constitutive behavior into our FEM code we would need to modify the code at hand (ANSYS) by writing a custom user material (USERMAT) subroutine based on the analytical representation for DED. However, the process of writing custom USERMAT is cumbersome and time consuming [16]. A relative new technology in its commercial form but with many years of research and development experience is providing the opportunity to solve this problem in a very efficient and economic manner. This is the Z-mat set of tools and it is briefly described below.

The Z-Mat toolset and environment

The development of advanced constitutive equations has been one of favorite research topics in the French School of Mechanics of Materials. After years of research on this area, a large base of constitutive models have become available along with a robust integration methods and advanced coefficient identification procedures. A commercialization of this technology was established by the joint effort among Transvator, Centre des Materiaux de L'Ecole des Mines de Paris and NW Numerics, Inc – a Seattle Washington company and although originally was targeted for ABAQUS [17] users, it has recently become available for ANSYS as well. The main modules of this technology are:

Z-mat is a dynamic library that extends the material modeling capabilities of ANSYS and ABAQUS, and provides a more flexible, object-oriented interface for developing user models of constitutive behavior. The source code of this product includes over 75K lines of C++ that implement various material models providing a very flexible set of constitutive equations. Many models are highly modular allowing the user to combine different "material model building bricks" to construct a new model dynamically. Many thousands of combinations are possible with application for metals, polymers, crystals, porous inelasticity (densification and damage), continuum damage mechanics, soil and rocks, and anisotropic materials. The nature of the library also allows all these models to be simultaneously available from a centralized location and the user is not obligated to copy a large usermat.f file to each project directory. Due to its modular design, the user can build new material models simply by expressing a material specification in the Z-mat input file in terms of existing combinations of flow rules, yield functions, and hardening rules. For example, plasticity-viscoplasticity does not exist as a predefined model; it can instead be fabricated in the input file, by the user, who can combine the simultaneous action of time-independent and viscoplastic strain components.

However, the most important feature of Z-mat is that it is not just a material model user routine library, but a whole suite of software with tools for simulating basic stress-strain behavior efficiently, fitting material coefficients to experimental data, interfacing with FEA software, and doing post processing. With all the complex capabilities, NW Numerics Inc. backs the software with exceptional (essentially consulting level) technical support standard with the software. Below are some of these tools.

ZebFront is a high-level material programming language. More advanced users will be interested in programming additions to the library, which is particularly simple via the use of the ZebFront pre-processor language. This language provides constitutive equation oriented data management commands on top of C++. Gives simplified access to integration methods (Runge-Kutta and implicit modified midpoint method), and interfaces with the many utility classes used throughout the library, which can be used as

building bricks for fast prototyping of new models. The combination of Z-mat with ZebFront have the potential of becoming one of the easiest ways to implement USERMAT applications, from a very high level object oriented programming point of view. The C++ foundation for the library also directly provides for the seamless integration of user extensions, appearing as if they were in fact part of the original library. Many user extensions can exist simultaneously, thus simplifying version control/management and end use.

Z-sim is a small simulator, allowing the user to load any representative volume element (RVE) in terms of mixed stresses and strains instead of forces and displacements. This allows for fast simulation of material tests without the use of FEA. It should be noted here that the material model code is shared 100% between the simulation and the FEA. The module includes functionality for plotting yield or damage (actually any potential participating in the material model) in stress space, at different points of the loading history.

Z-optim is an optimization module that includes several classical methods such as SQP, simplex or Levenberg-Marquardt, as well as genetic algorithms. Integrated with Z-sim, this module is a powerful tool for the identification of materials parameters, while keeping exactly the same user interface as Z-mat and Z-sim.

It is apparent from these descriptions that the existing capabilities in Z-mat are very extensive and dynamic, and they enable its usage as an idea development platform. However, the most important features of Z-mat that make it uniquely qualified for the task of automating the process of constructing a USERMAT routine are:

- **External variable storage:** Z-mat can now use an external database file for the state variables. This feature allows any number of state variables to be used with Z-mat breaking the barriers presented by different codes (e.g. ANSYS, Cosmos and ABAQUS).
- **Ability to run Fortran USERMATs:** Z-mat has a "wrapper" behavior that can be used to run Fortran USERMAT code within the Z-mat platform. This is primarily useful for using the Simulation/Optimization programs directly on those existing programs.
- **Ability to automatically create ZebFront scripts:** Using any scripting language (PERL, PYTHON, TCL/TK etc) users can complete the material modeling automation by computing instead of writing the ZebFront scripts that specify the material model.

Integration of Z-mat with ANSYS

Figure 5 below shows schematically some of the ways that Z-mat works with ANSYS (applicable to other ports as well), including separate input for the material, scripts for running ANSYS, the Z-mat constitutive library along with custom user extensions, and the extra Z-set modules such as simulation and optimization.

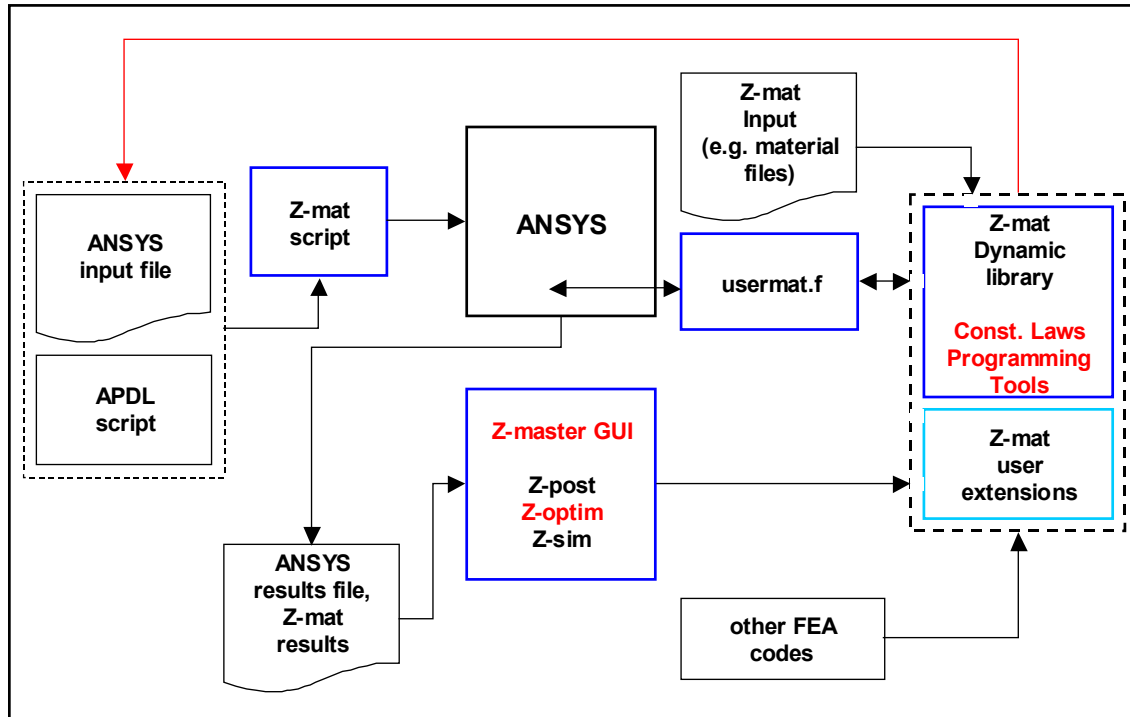


Figure 5 - Z-mat toolset integration with ANSYS

All the blue lined blocks in this diagram are parts of the Z-mat environment. The user will have to setup and execute the Z-mat script instance that is appropriate for his/her problem in addition to the Z-mat input file that contains the definition of the constitutive law either as a reference to an existing law in the library or as a specification for a synthesis of constitutive laws via the constitutive laws programming tools available in Z-mat. The block labeled “usermat.f” is not an actual USERMAT -as defined by the ANSYS documentation [7]- that is created once and linked with the ANSYS object code. Although it complies with the USERMAT specification it is rather a generic routine stub that allows the connection (passing of variables) of the constitutive laws as they are perceived by ANSYS, with their equivalent representation within the dynamic constitutive toolset offered by Z-mat. This way the user can be paying attention to the mathematical representation of the constitutive law and rely on the Z-mat-USERMAT-ANSYS bridge for the programming implementation that is being taken care by Z-mat automatically.

The process of running Z-mat with ANSYS entails launching a Z-mat script with the problem name. The script sets environment variables for linking with the library, and launches ANSYS. ANSYS in turn calls Z-mat in order to compile user materials defined in the Z-mat input file. When Z-mat is called to compile, there is actually nothing to do, except copy the Z-mat “stub” Fortran object file (pre-compiled) of the generic USERMAT to the project directory. After seeing that a USERMAT program was compiled the script launches Z-mat again to link. This time, the libraries sent by ANSYS are linked with the Z-mat libraries and the stub USERMAT file, and then copied to a temporary directory by ANSYS, at which point the problem starts.

When ANSYS finds a USERMAT, it passes the “name” of the material given in the input file to the USERMAT subroutine. It is thus possible to utilize multiple materials by using the name as a means to switch between routines. However, Z-mat uses this name as an external material file thereby letting ANSYS have access to a much larger and more robust method of data input. It is worthwhile to emphasize here, that the dynamic input structure of Z-mat files could never be possible with the classical USERMAT approach employed by the ANSYS development system.

Design Optimization Approach for Constitutive Behavior Characterization

The ground has been prepared to consider that the combination of Z-mat and ANSYS technologies allow us to extend the idea of design optimization beyond that which is applied for determining shape and other geometrical features of the model or material constants of generic constitutive models. In fact, now we can be thinking of a design optimization methodology that will be identifying the constitutive behavior model as well as the specific values of the free coefficients that participate in this model. Although these could be formulated as a two level staggered approach in design optimization, for the sake of generality we will be referring to both of these goals as “constitutive model characterization”. A verbal statement of the constitutive behavior characterization problem would be: *Given that there are plenty of experimental data documenting the kinematic response of a structure made out of a particular material system, determine the constitutive response model of the material that can best reproduce the observed experimental behavior by using a design optimization framework.*

In general, optimization problems are formulated in Z-optm in the standard form where the task of minimizing,

$$F = \frac{1}{2} \sum_{i=1}^N w_i (f(x, t_i) - y(t_i))^2 \quad (3a)$$

by changing $x \in S$ such that

$$g_j(x) \leq 0, j = 1, n_g \quad (3b)$$

has to be performed.

F is the cost or objective function (scalar), g is a vector of constrains, x are the parameters to be optimized, t_i tags the experiment (experimental point increment, experiment number, time tic, etc), and w_i is the weight associated with experimental point i . A variable x (set of parameters) such that $g_j(x) \leq 0, j = 1, n_g$ represents a feasible point. The default cost function F in Z-optm, is the least-square distance between experiments and simulations, and constraints g are used to bound and/or relate parameters with each other. However, Z-optm can also deal with other optimization methods.

There are two main categories of optimization methods. Global optimizers seek x^* such that

$$F(x^*) < F(x), \forall x \in S \text{ and local optimizer look for } x^* \text{ such that}$$

$F(x^*) < F(x), \forall x \text{ such that } \|x - x^*\| < \epsilon$. Typically, local methods iterate from a set from a set of variables x in the search space S to another, based on information gathered in the neighborhood of x . Zeroth order optimizers use exclusively the values of F and g . First order methods also employ $\text{grad}F$ and $\text{grad}g$, second order optimizers use the hessian determinants (or their approximation) of F and g . Global optimizers typically rely on pseudo-stochastic transitions in the search space (i.e. random hill climbing with reversal) in order to be able to escape local optima. An important difference between local and global optimizers, is that global optimizers are slower to convergence, but offer grater guarantees on the quality of the final solution produced. In many cases, convergence of global optimizers can be so slow that a solution cannot be obtained in a reasonable time period of execution. Another taxonomy for optimizers is based on the methodologies employed for handling the constraints. There are those that explicitly handle constraints like the state of the art SQP and those that do not (Levenberg-Marquardt or least squares, Simplex, evolutionary algorithms) [17].

The approach that is being advocated here as a surrogate to the traditional described in previous sections, is schematically described in figure 6 in terms of the participating modules and applications and their data interconnectivity as a flowchart.

It is clear that the Z-optm module will play a central role in our approach. While it can be interfaced with any external software that accepts ASCII input files, it is particularly well suited to application as a material coefficient determination (CBC) tool. Optimal coefficient sets are obtained by minimizing the total error between numerous reference curves (experimental results documenting kinematic structural behavior) and

simulated results. This method gives the best comprehensive fit of the material data while increasing confidence due to the numerous actual experimental data that contribute to the search for an optimal set of coefficients. The optimization loop is represented in figure 6 by the data path represented by red arrows. The optimization process is controlled by the error minimization between the actual data and the simulated response and starts with an initial guess of all constants involved. The final values of these constants will be the outcome of the process.

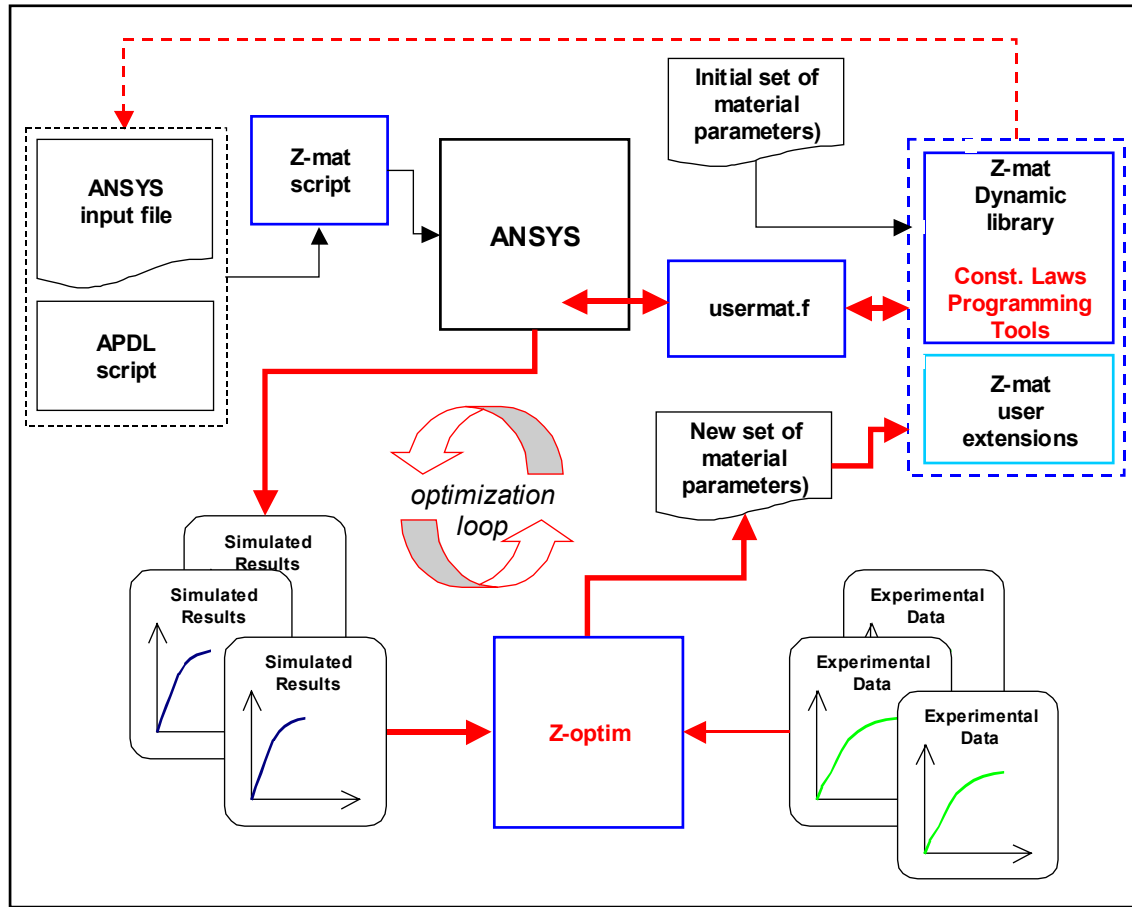


Figure 6 - Z-mat and Z-optimize based constitutive characterization

However, prior to deciding on initial values of the participating coefficients we have to deal with the issue of what is the analytical representation of the constitutive behavior that these constants are a part of. Also, in order to address the issue of how ANSYS would be computing simulations of our experimental data we have to first address the issue of the starting material behavior form that we will encapsulate in Z-mat to be passed via the USERMAT stub to ANSYS. This would in turn require that we assume the existence of an equational representation for the constitutive response. This form will have free coefficients (constants) to be determined from the employed methodology. We currently envision that there are at least three potential avenues to establishing a mathematical representation with free coefficients that could fit this requirement:

- **Heuristics on past experience.** Exploit heuristic rules based on prior experience on how experimental kinematic (load-displacement) behavior relates with known mathematical representations, and attempt to select one of the known forms to see how well it can serve this purpose for the particular application. Certainly, these representations may be based on particular physical behavior (flow, crazing, cracking, microcracking etc) that is observable in the test specimens in addition to their kinematic behavior or even desire to adhere to first principles (such as thermodynamics and conservation laws).

- **Internal Variable Representations.** Utilize state variables that although may not be physically observable or/and measurable they may be useful in describing material state and practical in handling the mathematics of state evolution. Examples would be the damage variables in the various isotropic and anisotropic damage models. Chances are that however useful a model of this category may be, it may still violate thermodynamic principles like the Clausius Duhem inequality for entropy production by a material system.
- **General Polynomial.** Assume the existence of a general polynomial of nth order. Its variables would be the state variables of choice, while its coefficients will be holding the material specific information to be determined. Although this approach is blind to any physical or axiomatic considerations, it has the power of the “brute-force” approach.

Assuming the existence of a potential function with two parts, one for the elastic part of the behavior and one for the inelastic, one would be an example of a PMC damage behavior encapsulation that would certainly fit in the first category above. For our case this situation could be represented by:

$$\phi(\tilde{\mathcal{E}}, m) = \phi_{el}(\tilde{\mathcal{E}}, \tilde{c}) + \phi_{inel}(\tilde{\mathcal{E}}, \tilde{c}) = \left[\frac{1}{2} C_{ij}^{kl} \varepsilon_{ij} \varepsilon^{kl} \right]_{el} + [D_{ij}^{kl} \varepsilon_{ij} \varepsilon^{kl} + E_{ijmn}^{kl} \varepsilon_{ij} \varepsilon^{kl} \varepsilon_{mn} + \dots]_{inel} \quad (4)$$

where $\tilde{\mathcal{E}}, \varepsilon_{ij}$ are the vector and the contracted representations of the strain tensor, and $C_{ij}^{kl}, D_{ij}^{kl}, E_{ijmn}^{kl}, \dots$ are the elastic tensor, and the various fourth and higher order tensors containing all constants responsible for the material's damage behavior.

Assuming the existence of an anisotropic elastic-degrading (damage) constitutive law of the form,

$$\phi(\tilde{\mathcal{E}}, m) = \phi_{el}(\tilde{\mathcal{E}}, \tilde{c}) + \phi_{inel}(\tilde{\mathcal{E}}, \tilde{c}) = \left[\frac{1}{2} C_{ij}^{kl} \varepsilon_{ij} \varepsilon^{kl} \right]_{el} + \left[\frac{1}{2} D_{ij}^{kl} \varepsilon_{ij} \varepsilon^{kl} \right]_{inel} \quad (5)$$

where D_{ij}^{kl} is fourth order tensor containing all constants responsible for the material's damage behavior.

This case would fall in the second category of models. Finally assuming the existence of a general polynomial of the form,

$$\phi(\tilde{\mathcal{E}}, m) = \phi(\tilde{\mathcal{E}}, \tilde{c}) = c_1(m) \chi_1(\tilde{\mathcal{E}}) + c_2(m) \chi_2(\tilde{\mathcal{E}}) + \dots + c_n(m) \chi_n(\tilde{\mathcal{E}}) \quad (6)$$

would fall in the third category of mathematical representations for constitutive models. The coefficients c_i are to be determined and are uniquely associated with the material system they stand for. The fact that equation (7) is identical to equation (2) is based on the idea that the traditional approach described earlier was also intended to be of a most general applicability.

We are planning to eventually apply this scheme for all three cases. However, as it is evident from equations (5) and (6) it is obvious that the process can also be applied for backing out the elastic constants that constitute the components of the C_{ij}^{kl} tensor by dropping the rest of terms.

A Special Case: Data driven Determination of the Elastic Properties

We have applied the process described above, for the case of a data set corresponding to IPLS tests for the AS4-3501-6 PMC material system. The initial elastic properties [19] that we started with and the final properties resulting from the optimization are shown in table I. Since we tested this procedure initially on all datasets the case with the in-plane rotation were used with the grip slippage not accounted for. After taking those cases out of the input set and utilized those cases that were free of grip slippage we obtained the numbers in the third row of table I. On a 360 MHz Sun Ultra 5, a complete optimization sequence required 10 hours.

Table 1 - Initial and final values of elastic properties

	E_{11} (psi x 10e6)	E_{22} (psi x 10e6)	G_{12} (psi x 10e6)	ν_{12}
Initial values	20.0	1.5	1.0	0.27
Ending values (grip slippage)	0.2	0.782104049	0.08	0.45
Ending values (no grip slippage)	19.2	1.23	0.915	0.32

For this case, the path through the USERMAT stub in figure 6, is not necessary. Only the elastic properties of the original ANSYS model need to be changed at each optimization iteration. This is accomplished by following the dashed line path on the top of figure 6.

The model was created by an APDL script and is shown in figure 7. The elements used was SHELL63 from the ANSYS library. The model was constructed with boundary conditions that allow direct implementation of the displacements applied on the actual specimens by IPLS and in the postprocessing section of the macro the reaction forces at the boundaries are computed to be used for constructing the simulated load-displacement response. It is important to realize that all data have been used for all for laminate constructions [2-4] of +/- 15°, 30°, 60° and 75°. The 15 loading paths per laminate configuration multiplied by two for each of the two specimens used (for statistical control along each loading path), generate a total of *4 (layups) x 15 (loading paths) x (2 specimens) = 150 data sets per material system*.

Since we average the data for the specimen pairs, we end up utilizing 75 derived data sets that are more than enough to construct an overdetermined system of equations participating in the optimization scheme.

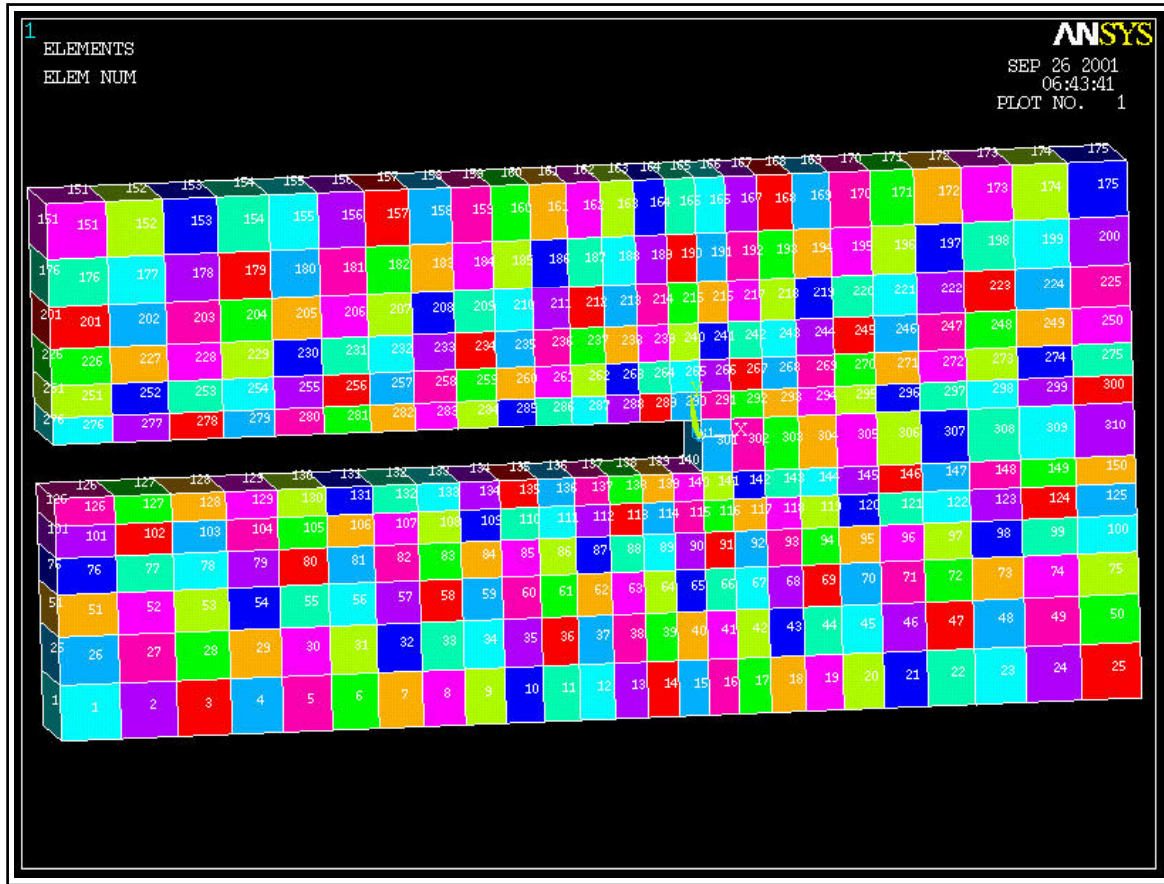


Figure 7 - ANSYS model of IPL's single notched specimen

Figures 8 through 10 show characteristic representative curves of the boundary displacements for loading paths 2 (closing displacement along y axis), loading path 8 (shearing motion parallel to the x-axis) and loading path 14 (opening displacement along positive y axis). The corresponding forces are shown in figures 11 through 13. In all of these graphs there are two sets of curves one for the experimental data and one for the predicted (the shorter ones) data. The simulated responses are presented for only the first twelve points of each loading path since at this stage the optimization process was only applied for extracting the elastic constants of the PMC system and therefore it was anticipated that only the first experimental points would correspond to the elastic part of the specimen's behavior.

As it is anticipated the predicted displacement curves are following almost identically the experimental curves (figures 8-10) since they have been formed as input boundary conditions in our ANSYS model of the specimen.

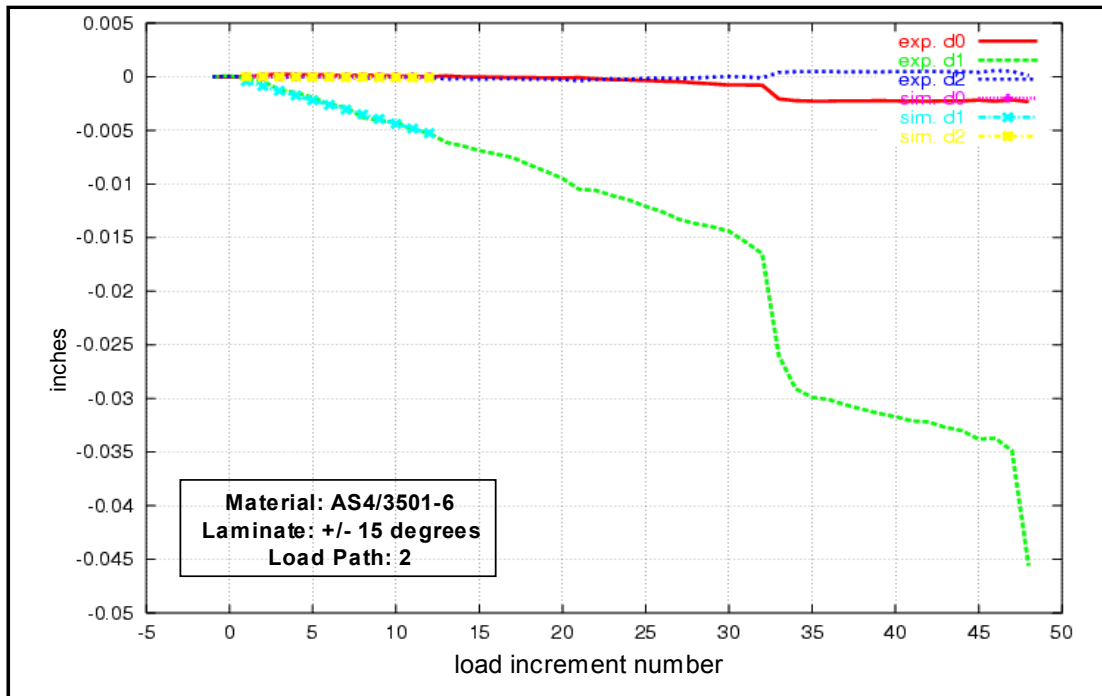


Figure 8 - Typical experimental and simulated displacement history for loading path 2.

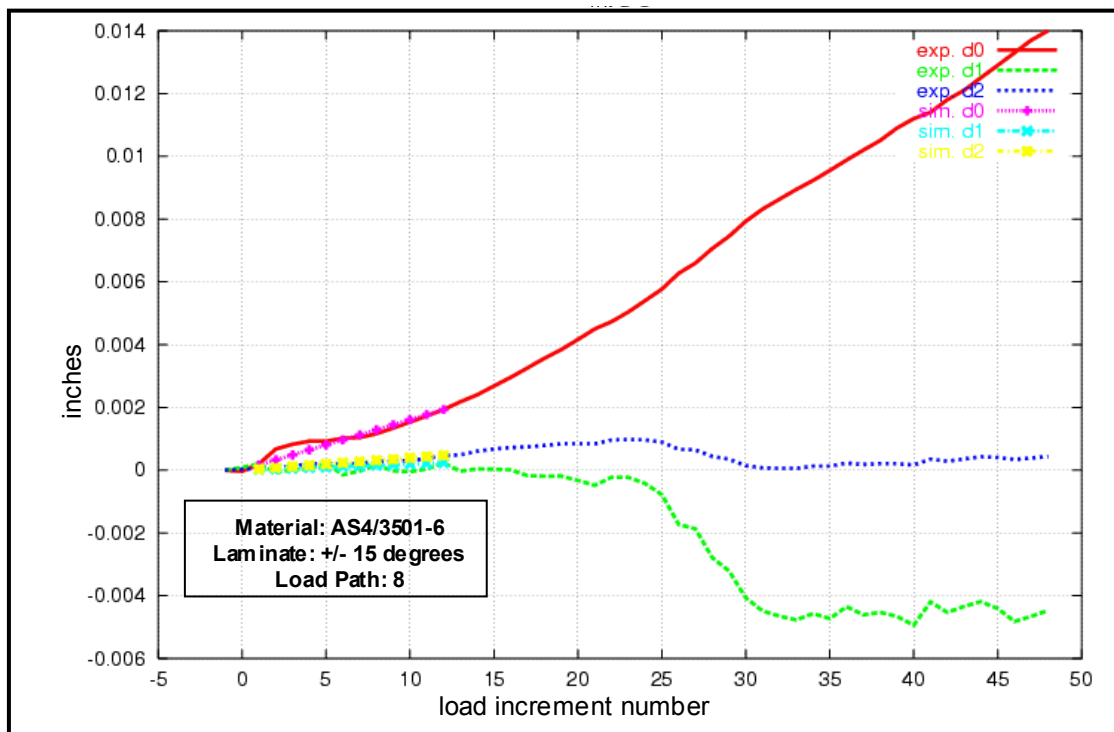


Figure 9 - Typical experimental and simulated displacement history for loading path 8.

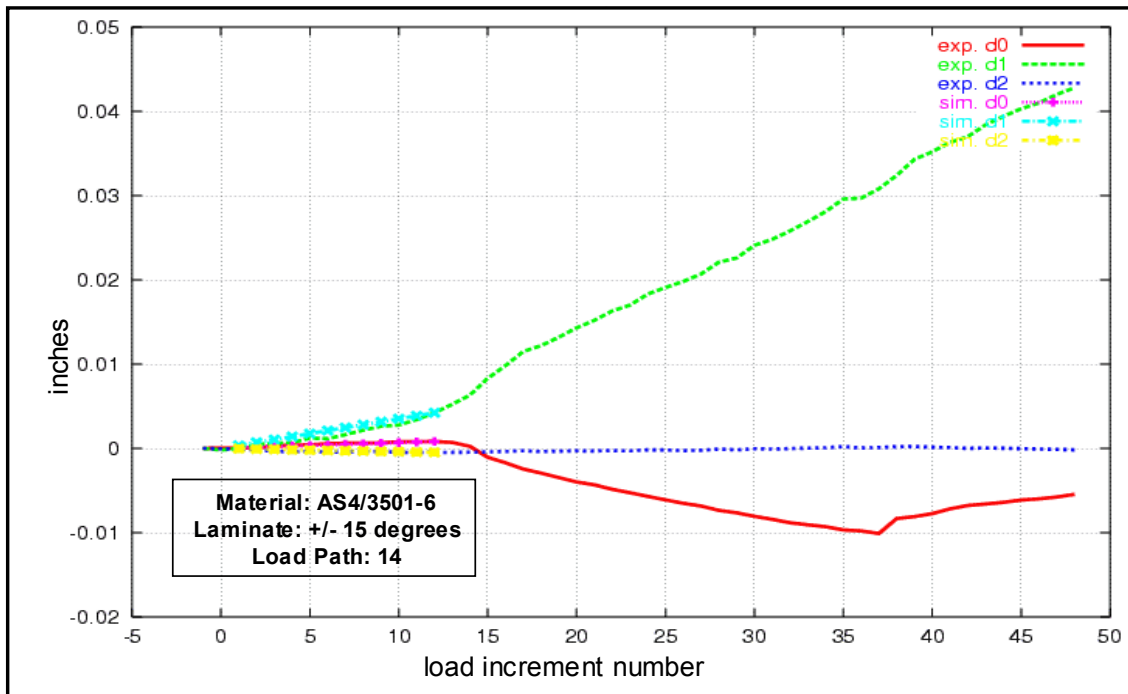


Figure 10 - Typical experimental and simulated displacement history for loading path 14.

However, the forces start well in the beginning, by matching almost always the first points of their corresponding experimental curves. Subsequent PMC softening makes the experimental curve presenting deviations as the imposed displacement increases for each subsequent loading point.

Figures 8 through 13 present the difference between the actual and the simulated load-displacement behavior of the specimen. During this stage the elastic constants used at the simulation are the initial ones as given by the first row table I. The corresponding curves for the derived elastic properties presented in the second row of table I, are not worthwhile presenting because they are still very similar to the initial ones. This fact indicates that one has to incorporate a non-linear constitutive behavior law to have the simulation further approximate the experimental data. This task will be completed in the near future as a direct consequence of the present effort.

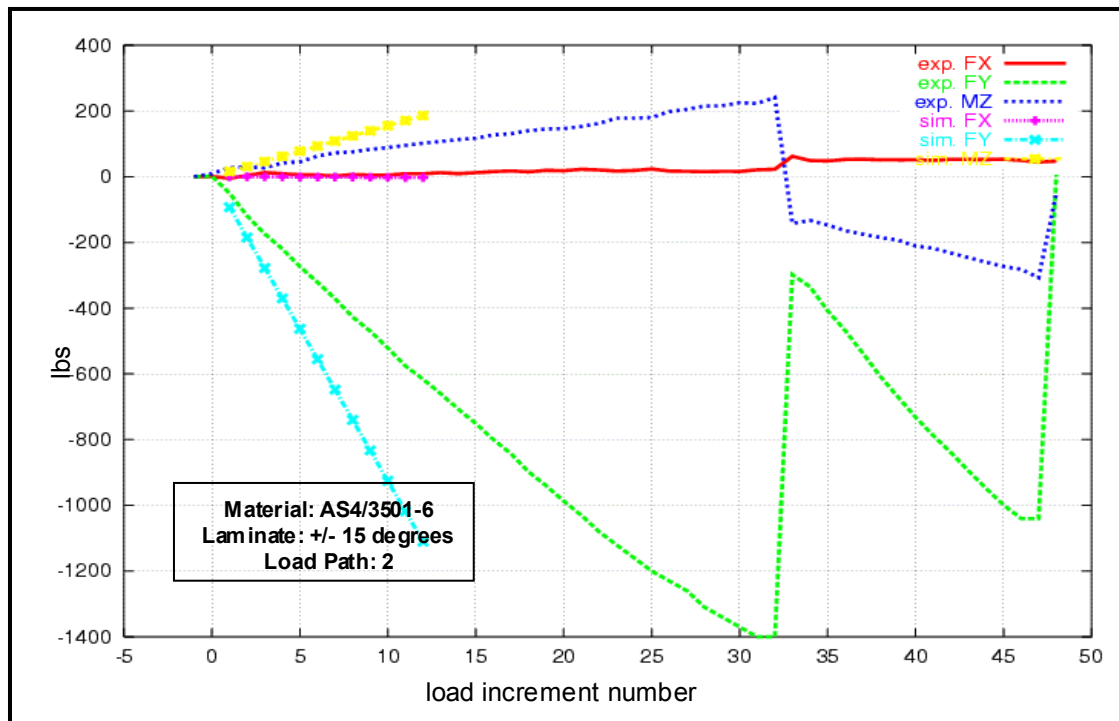


Figure 11 - Typical experimental and simulated force history for loading path 2.

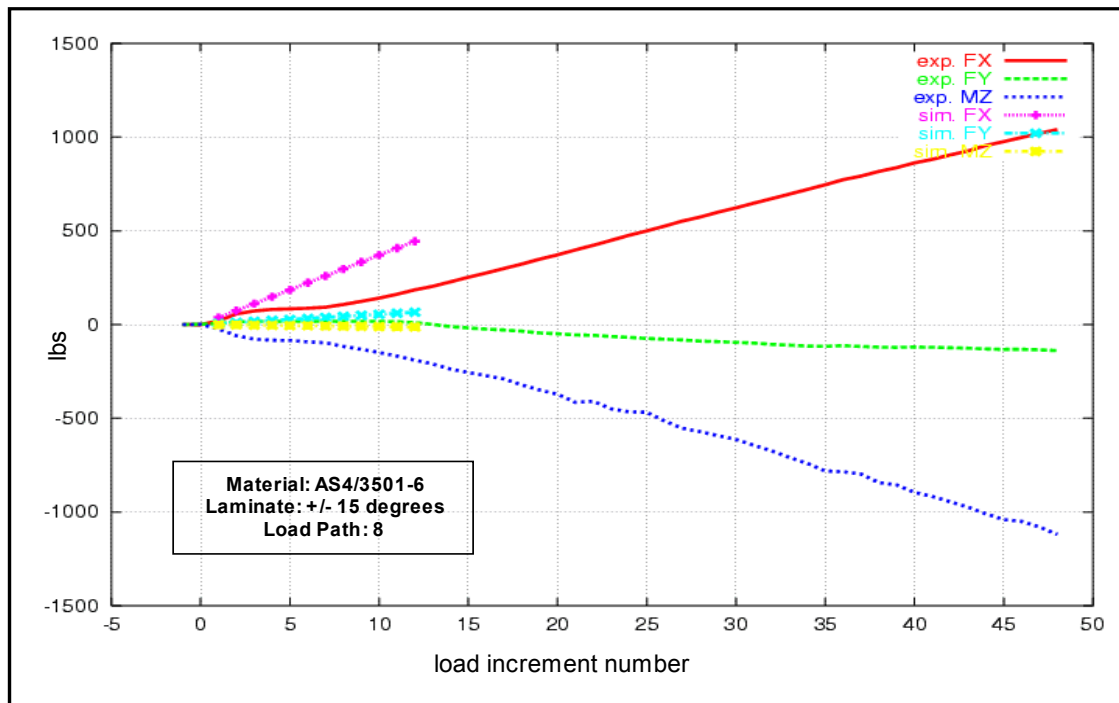


Figure 12 - Typical experimental and simulated force history for loading path 8.

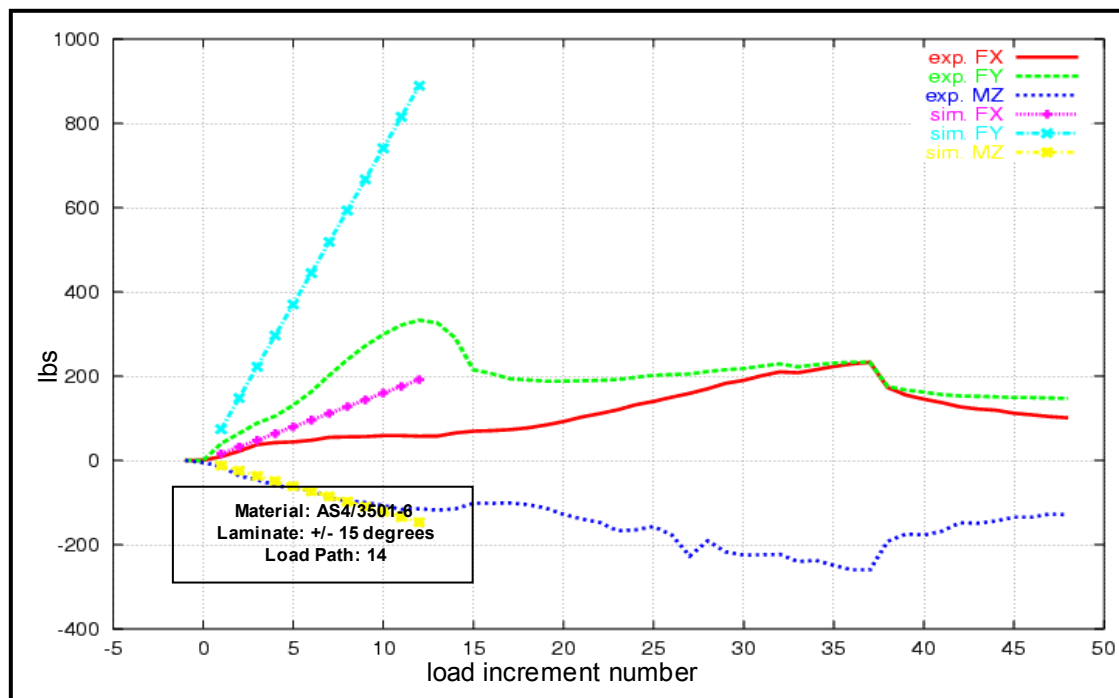


Figure 13 - Typical experimental and simulated force history for loading path 14.

Concluding Remarks

A very powerful combination of tools allows for the dynamic and automated constitutive behavior characterization from experimental data. It is very encouraging that there is no need for very specialized knowledge to use these tools based on Z-mat and ANSYS technologies. It is anticipated that the accuracy and the build-in verification (due to the fact that they are constructed to match massive experimental data) that constitutive models built according to the described approaches, will drastically increase the confidence of end users for various kinds of applications. This technology along with the anticipated user confidence has the potential to brake open for substantive application and exploitation many from the (virtual) design and prototyping of structures, to material synthesis by design as well as material qualification and certification.

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