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An Inverse Method for Analyzing Defects in Heterogeneous Materials

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ABSTRACT
Evaluation of defects in heterogeneous materials, such as cellulose-fiber composites, can lead to methods for improving strength. Full-field displacement measurement techniques, *e.g.*, digital image correlation and electronic speckle pattern interferometry, provide useful information by which defects can be evaluated. Inverse Methods (IM) have been used to determine material properties from full-field displacement data. In homogenous materials, the resulting system of equations relating displacements with applied load and constitutive properties is overdetermined and is solved with traditional least squares methods. However, heterogeneous materials create an underdetermined system that cannot be addressed in the same way. Numerically simulated heterogeneous, orthotropic materials were evaluated in a 2-D finite element model, and the resulting nodal displacements were used as input to an IM algorithm. The algorithm determined local moduli, E_x and E_y, with errors, ranging from 9% to 20%. Errors in calculated G_{xy} were greater. Techniques for reducing error are provided. Simulations suggested IM can be an important tool in defect evaluation given full-field displacement measurements.

INTRODUCTION

All practical engineering materials contain strength-reducing defects. Defects increase local stresses above far-field applied stress through disorder, discontinuities, and material variability. For many years, measurement of strength reduction was a primary method of defect detection. In general, defects lower strength by concentrating stresses to levels that can be an order of magnitude greater than far-field stresses. Size, location, and frequency of defects in crystalline and ceramic materials have been an area of active research for many years. Hull and Bacon [1] described the stress fields caused by a variety of defects in crystalline solids.

Defect analysis of materials containing long-chain polymers, such as cellulose fibers in paper, has concentrated on fracture behavior [2-4]. However, papermaking also creates defects through variations in fiber alignment, fiber-to-fiber bonding, distribution of fiber lengths, and other parameters. As the density of native cellulose approaches 1500 kg/m^3 and paper density ranges from 600-800 kg/m^3, a large amount of void space is present that generates geometric defects with a range of sizes and shapes. As in crystalline materials [5], these defects can be detected through stress-distribution analysis.

One method of evaluating stress distribution is the use of inverse methods (IM). Avril and Pierron [6] reviewed several IM approaches and showed their general equivalency. IM can be generally described as the iterative adjustment of parameters in a numerical model, usually a FEM (finite element method) model, to minimize the

difference between an experimentally measured quantity and the numerically calculated quantity. For example, adjustable parameters may be constitutive properties and the measured quantities may be displacements.

By comparing FEM calculated out-of-plane displacements with those measured by shadow moiré, Le Magorou *et al.* [7] used IM to determine bending stiffness in composite wood panel. Molimard *et al.* [8] evaluated E_{xx}, E_{yy}, ν_{xy}, and G_{xy} of a composite material by minimizing the difference between moiré-measured displacements and those predicted by FEM in a perforated tensile plate. Similarly, Genovese *et al.* [9] used IM procedures to evaluate a truss system and a composite plate. Each of these references incorporated a specific type of IM entitled FEMU-U (finite element method updating–displacement).

With FEMU-U, the r.m.s. (root mean square) of displacement differences, also called a cost function, between measured values and those predicted by FEM are minimized by iteratively changing constitutive parameters in the FEM model. FEMU-U is attractive because displacements are first-order outputs of high-resolution full-field techniques of DIC and ESPI. Strain, a second-order output, has greater noise associated with numerical differentiation.

A common feature of these earlier investigations [7-9] is that only homogeneous materials were evaluated. The resulting system of equations was overdetermined. In 2-D models, the degree of freedom is (number of nodes) x 2 – (number of constitutive parameters) – 1. For homogeneous, isotropic materials, the number of constitutive parameters is two (E, ν); for homogeneous, orthotropic materials, the number of constitutive parameters is 4 (E_1, E_2, ν_{12}, G_{12}). For either case, the number of degrees of freedom is large and the problem has a unique solution based on minimizing least squares of the chosen cost function.

Quasi-heterogeneous material systems have been evaluated by Sutton *et al.* [10], who evaluated a weld-zone between two isotropic materials, and by Avril *et al.* [11], who identified the stiffness ratio between a high modulus spherical inclusion within a low modulus material. In these cases, a large portion of each specimen was homogeneous and isotropic.

Contrasted with isotropic cases, the system of equations associated with evaluating the constitutive parameters of heterogeneous, orthotropic materials is underdetermined in that there are many more parameters to evaluate than available inputs. A heterogeneous, orthotropic FEM model consisting of 100 four-node quadrilateral elements, arranged in a 5 x 20 array, has 126 nodes (252 displacement inputs) and 400 constitutive parameters to be determined. Underdetermined systems have an infinite number of solutions; the conventional least squares solution of an underdetermined system minimizes the appropriate cost function using the smallest value of constitutive parameters.

Heterogeneous, orthotropic models are important in defect analysis of composite materials. In fibrous composites like paper, defects can be attributed to items such as locally varying orthotropy ratios, fiber misalignment, low weight and poorly bonded regions, non-uniform fiber length, and incorporation of foreign materials. Each of these defects alters the surrounding stress field, creating regions of tensile and compressive stress concentration. Knowledge of local stress combined with local constitutive parameters provides the basis for defect analysis.

The goal of this work is to numerically simulate defects in heterogeneous, orthotropic materials and to use those simulations to evaluate the effectiveness of FEMU-U in determination of local constitutive parameters. These simulations reflect worst-case scenarios; material properties that limit variability, such as material characteristic length, were not incorporated in the simulations. Parasitic displacement noise was not included in this exploratory evaluation. The resulting system is underdetermined, but approaches are suggested for improving model conditioning.

Here defects are defined by any combinations of disorder, discontinuity, or variability that cause local stresses to exceed far-field applied stresses. This work describes two simulations: (1) a simulation to produce defects through local constitutive property variability and (2) a simulation to incorporate nodal displacements of a uniaxial tensile and biaxial tensile specimen in a FEM model from the first simulation in a FEMU-U algorithm to determine local constitutive properties.

METHODS

Evaluation of FEMU-U for heterogeneous materials was accomplished through numerical simulations of five parameters known to be associated with defects in paper materials and IM analysis of 100 randomly selected simulations. The five parameters included (1) principal elastic modulus, E_1, (2) COV (coefficient of variation) of E_1, (3) orthotropy ratio, $R = E_1/E_2$, (4) COV of misalignment angle, θ, between the principal material direction and direction of load application, and (5) COV of density, ρ. The following pseudo-code generates material properties for 100 elements as input for a FEM model.

→ *Let* E_1 *vary from 4 GPa to 10 GPa in 0.5 GPa increments [13 cases]*
  → *Let* COV(E_1) *vary from 10% to 40% in 10% increments [4 cases]*
  → *Generate 100* E_{11}*s randomly from normal distribution with mean* E_1 *and* COV(E_1)
    → *Let R (orthotropy ratio) vary from 2.0 to 5.0 in 0.25 increments [13 cases]*
    → *Generate 100* E_{22}*s randomly from normal distribution with mean* E_1/R *and* COV(E_1)
      → *Let* COV(θ) *vary from 10% to 40% in 10% increments (with* COV(θ) *evaluated at* θ*=45°[4 cases] (*see following discussion in text)*
      → *Generate 100* θ*'s randomly with mean 0° and* COV(θ)
        → *Let* COV(ρ) *vary from 10% to 40% in 10% increments [4 cases]*
        → *Generate 100* ρ*'s randomly with mean 1.0 and* COV(ρ)
          → *Let* $\nu_{12} = 0.23$ *(common for cellulose materials)*
          → *Let* $\nu_{21} = \nu_{12} \cdot E_{22}/E_{11}$ *for each of 100 elements*
          → *Let* $G_{12} = \sqrt{E_{11}E_{22}} \Big/ \left[2\left(1+\sqrt{\nu_{12}\nu_{21}}\right)\right]$ *for each of 100 elements* (see [12])
          → *Let* $[E'_{11}, E'_{22}, G'_{12}] = \rho \cdot [E_{11}, E_{22}, G_{12}]$
          → *Calculate* E_x, E_y, ν_{xy}, G_{xy} *from transformation of* $E'_{11}, E'_{22}, \nu_{12}, G'_{12}$ *with* θ *for each of 100 elements*

*Calculation of θ: 100 θ were randomly generated with a mean of 45° and the specified COV and 45° was subtracted from each of the 100 θ values.

The pseudo-code produces 10816 heterogeneous simulations, each with 100 elements. These simulations represent worst cases because large variations in material properties are allowed in adjacent elements. Such cases are justified by the large COV(ε), as great as 40%, measured by researchers [13-15] during tensile testing. Material characteristic length or correlation distance, which describes how rapidly material properties vary in space, is not included.

Here K_t, tensile stress concentration factor, is defined as the ratio of FEM-calculated element stress in the direction of far-field stress to far-field stress. K_c is defined as the ratio of FEM-calculated element stress in the direction orthogonal to far-field stress to far-field stress. A homogeneous, linear elastic tensile specimen has K_t equal to unity and K_c equal to zero.

Each of the 10816 heterogeneous simulations was used as input for two FEM models, shown in Figures 1a and 1b. The long model dimension corresponded with the y-direction because 2-direction properties are generally the most critical in applications involving paper materials. FEM analysis was performed within ANSYS® using PLANE42 (4-node quadrilateral) elements and an orthotropic material model. Nodal displacements were used as input to the FEMU-U solver. Parasitic noise was not added to nodal displacements but has been addressed in other simulations [6].

The particular inverse method used here is FEMU-U, finite element model updating via displacement gap. Through an iterative process that determines new constitutive parameters, the displacement difference between the simulation-produced nodal displacements and FEM nodal displacements is minimized. Nodal displacements come from the constitutive property variability simulations and are used as input to the FEMU-U algorithm.

The function to be minimized is

$$f(\hat{u}_{FEM}, P) = \|r\| \; where \;\; r = (\hat{u}^{Simulation} - \hat{u}^{FEM}) \tag{1}$$

where

$\hat{u}^{Simulation}$ = vector containing nodal u-, v-displacements determined by heterogeneous model simulation
$\hat{u}^{FEM}$ = vector containing nodal u-, v-displacements from FEM model
P = vector containing constitutive parameters, E_x, E_y, ν_{xy}, G_{xy}
$||r||$ = norm of r

Because Equation (1) is nonlinear with respect to P, iterative procedures are appropriate methods for minimization of $f(\hat{u}_{FEM}, P)$ and determination of P. LMA (Levenberg–Marquardt Algorithm) (*e.g.*, see [16]) is commonly used because it combines the benefits of Steepest Descent Method with Gauss–Newton Method. The LMA has the form

$$P_{i+1} = P_i - (J^T J + \lambda \cdot diag(J^T J)^{-1} J^T r \tag{2}$$

where

i = iteration number
J, J^T = Jacobian and Jacobian transpose, determined by backward difference, $J_{m,n} = \frac{\partial r_m}{\partial P_n}$; m = number of nodal displacements (number of nodes x 2 for planar models), n = number of constitutive parameters x number of elements (100 in this work)
λ = non-negative damping factor, adjusted each iteration step, adjusts between Steep Descent Method and Gauss–Newton Method.

The Jacobian, J, in Equation (2) is calculated by backwards finite difference. The primary disadvantage of LMA is the need for matrix inversion during each iteration. In most applications, reduced iterations compensate for the matrix inversion.

After calculating a new $P_{i+1}$the constitutive parameters are checked for validity, *e.g.*, a positive-definite stiffness matrix in the FEM model, and are adjusted if not valid. Invalid elements P_i are adjusted to global mean P_i. The validated $P_{i+1}$are inputs to a new FEM analysis and the resulting nodal displacements are used to determine f_{i+1}. If $f_{i+1} < f_i$, the constitutive parameters are updated, $P_{i+1} \rightarrow P_i$, λ is reduced by a factor of 10, and the next iteration begins. If $f_{i+1} > f_i$, then λ is increased by a factor of 10 and P_i is not updated. As $\lambda \rightarrow 0$, LMA becomes exactly the Gauss–Newton Method. Typically 10 iterations were required.

RESULTS AND DISCUSSION

Figure 2a compares maximum tensile stress concentration, K_t, and maximum absolute value of the compressive stress concentration, K_c, for each heterogeneous simulation used as input for the FEM model in Figure 1a. Compressive failure strength for cellulose materials is typically 25% of tensile failure strength for both 1- and 2-directions; therefore, the simulated defects appear sufficient to test the ability of IM to determine heterogeneous constitutive behavior. A randomly chosen 100-member subset of scenarios (shown in Figure 2b) was used for subsequent investigations.

The model system, as originally formulated, was underdetermined because it contained 400 unknowns (E_x, E_y, ν_{xy}, G_{xy} for each of the 100 elements) with 252 inputs (126 nodes with u-, v-displacements). A possibility to improve system conditioning is to increase node density, but ultimately this is not a practical solution. One would usually like to know local behavior at the smallest element size possible based on experimental measurement techniques. If a particular measurement technique can accurately provide displacement information within a 1-mm x 1-mm grid, a resulting FEM model using PLANE42 elements would have element size of 1 x 1 mm. An 8-node quadrilateral element, such as the ANSYS® PLANE82 element, would need to be 2 x 2 mm and the region over which the constitutive properties are determined for this element would be 4 times larger than for the PLANE42 element.

System conditioning was improved here following the example of other researchers, Avril *et al.* [17] for example, reduced the number of parameters by eliminating ν from iterations. This approach was employed here in that ν_{xy} was assumed to be a homogeneous 0.23, based on representative results from Baum *et al.* [18].

LMA requires two initial estimates of P in order to calculate J and begin iterations. Genovese *et al.* [9] evaluated the effect of initial estimates on the number of iterations using FEMU-U in an overdetermined system and found that poor initial estimates increased the iterations required for minimization, but minimization was eventually achieved. Although thorough evaluation of initial estimates is beyond the scope of this investigation, an informal

analysis showed lack of convergence for poor initial estimates, primarily because the rate of convergence was different for each of E_x, E_y, and G_{xy}. It was found that minimization could be achieved if the first initial estimate for each of E_x, E_y, and G_{xy}, was the same throughout and with each modulus estimated 2 times larger than expected. The second initial estimate assumed that each of the parameters was heterogeneous, with E_x and E_y approximated at their mean values with a COV of 10%, and randomly assigned to each of the 100 elements. The mean value initial guess for E_x and E_y was justified because these values are generated during the same experimental tests used to capture full-field displacements. The second initial estimate for element G_{xy} was calculated as in the pseudo-code, with ν_{xy} = 0.23, *i.e*,. $G_{12} = \sqrt{E_{11}E_{22}} \Big/ [2(1+\sqrt{\nu_{12}\nu_{21}})]$.

Figures 3a and 3b show some results of FEMU-U applied to 100 simulations of the uniaxial load model, illustrated in Figure 1a. Root mean square errors provide an estimate of global error and were calculated according to

$$\%RMS_e(P_i) = \frac{norm(P_i^{Simulation} - P_i^{FEM})}{\sqrt{number\ of\ elements} \cdot mean(P_i^{Simulation})} \cdot 100\% \tag{3}$$

where

P_i = one of E_x, E_y or G_{xy}

Some correlation appeared evident in Figure 3a between the errors of E_x and E_y; $\%RMS_e(E_x)$ increased with $\%RMS_e(E_y)$.This type of behavior was expected because error in E_x cannot be compensated in E_y. The converse is also true. Such an understanding has practical application in that usually some material behavior is known prior to evaluation. If an FEMU-U algorithm for an underdetermined system produces a result contrary to known behavior in E_x or E_y, all material parameters are likely inaccurate.

A similar correlation was not evident in Figure 3b. Errors in the calculation of G_{xy} were higher and had no general trend with errors in E_y. Shear-induced nodal displacement was minimal for the uniaxial loading in Figure 1a and was created by nearby property heterogeneity. Another factor increasing $\%RMS_e(G_{xy})$ was a poor initial estimate. Avril *et al.* [17] used an Iosipescu shear test for accurate determination of G_{xy} in a homogeneous, orthotropic material.

Simulations allowed freedom to investigate unrealistic test geometries, such as in Figure 1b. This geometry was included to determine if FEMU-U more accurately determines E_x, E_y, and G_{xy} with alternate loading configurations. Figures 4a and 4b show errors of moduli as determined with the biaxial load geometry. The errors were similar to those in Figures 3a and 3b. No significant improvement in E_x, E_y, and G_{xy} were observed.

It is encouraging to note that comparison of Figures 3a and 4a suggests that uniaxial testing is sufficient for E_x, E_y determination. However, accurate determination of local G_{xy} seems to require a test geometry with significant shear behavior.

Errors shown in Figures 3 and 4 may seem high considering the lack of parasitic noise in simulated nodal displacements. This type of noise was not introduced because it creates a specific length scale that can be accurately determined only when a specimen geometry and evaluation scale are determined.

Errors in moduli determination can be reduced by determination of ν_{xy}. In specific simulations with large orthotropy ratios, inaccuracy of ν_{xy} greatly increases errors in moduli. In applications, determination of local ν_{xy} may be important because locally negative values may exist.

We are working to improve the accuracy of FEMU-U in defect analysis in the following ways:

- Material correlation length—This length scale can be used to limit the gradient of moduli changes.
- Knowledge of defect location—Nodal displacements in the region of the defect can be weighted to improve moduli determination near that region.
- Moduli filtering—Similar to correlation length, filtering can be used to damp periodic large moduli fluctuations associated with displacement measurement errors.

CONCLUSION

Defect analysis of materials can be accomplished by the determination of stress concentrations within materials. Numerical simulations were performed to create a variety of heterogeneous models that exhibited tensile and compressive stress concentrations. Nodal displacements, as calculated by a heterogeneous, orthotropic FEM model, were used in a FEMU-U algorithm to determine its success in local moduli evaluation. The resulting system was underdetermined as it attempted to compute 300 moduli from 252 inputs. E_x and E_y, as determined by FEMU-U, had similar errors, from 9% to 20%. Calculations of G_{xy} had larger errors. Uniaxial and biaxial models had similar errors in moduli determinations. Some portion of the errors was attributed to the elimination of Poisson's Ratio in the FEMU-U algorithm.

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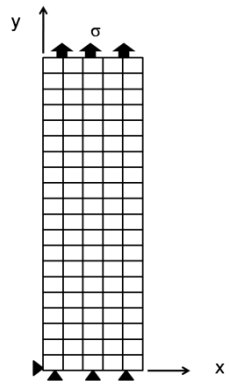

Figure 1a: FEM model for uniaxial loading.

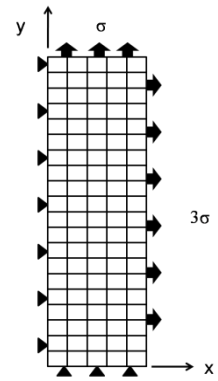

Figure 1b: FEM model used for biaxial loading.

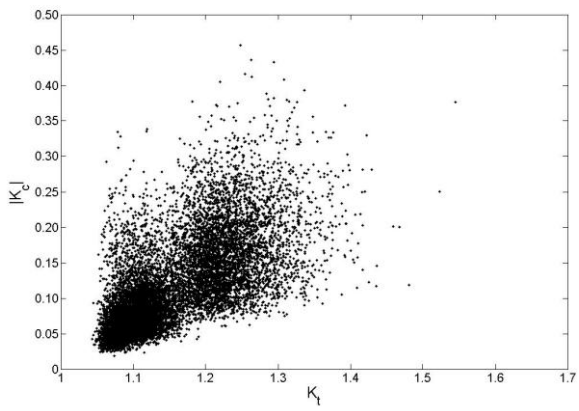

Figure 2a: Maximum tensile stress concentration compared to minimum compressive stress concentration for each simulation.

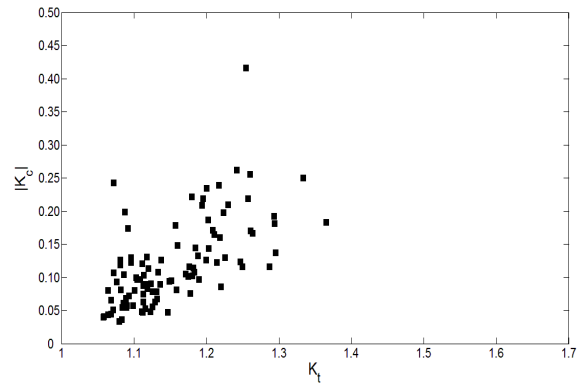

Figure 2b: A subset of 100 randomly chosen simulations from Figure 2a subsequently used for FEMU-U.

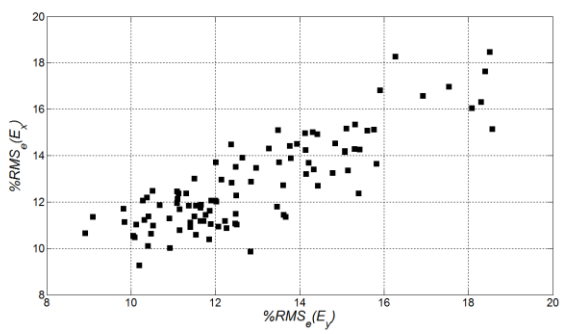

Figure 3a: Root mean square error of E_y and E_x for uniaxial loading, as a % of actual mean E_y and E_x.

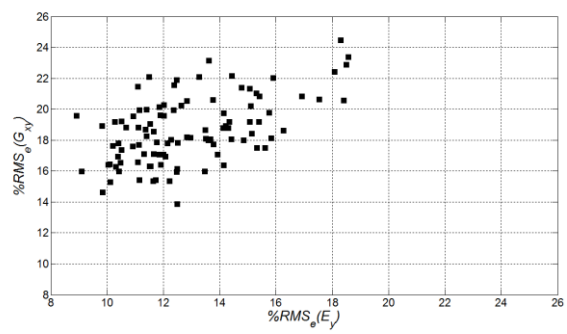

Figure 3b: Root mean square error of E_y and G_{xy} for uniaxial loading, as a % of actual mean E_y and G_{xy}.

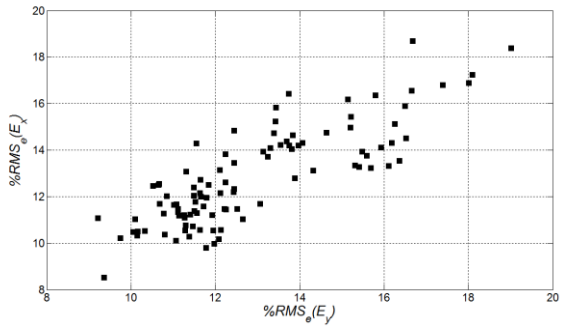

Figure 4a: Root mean square error of E_y and E_x for biaxial loading, as a % of actual mean E_y and E_x.

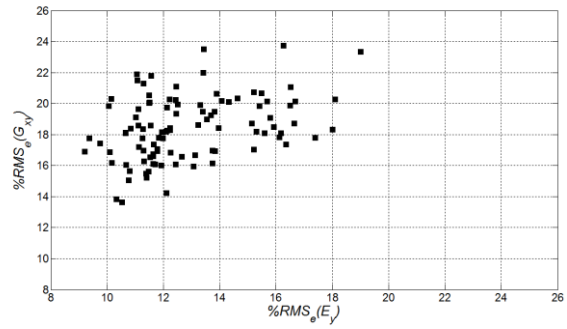

Figure 4b: Root mean square error of E_y and G_{xy} for biaxial loading, as a % of actual mean E_y and G_{xy}.

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