SCALABLE COUPLING OF TFA AND PARADYN ANALYSES FOR IMPACT MODELING OF 3-D WOVEN COMPOSITES

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Abstract: Two stand alone computer codes are coupled for conducting scalable computation of dual-scale impact analysis of 3-D woven composites. The first code, which works at a local level, used an RVE, i.e. a representative volume element, based transformation field analysis (TFA) for describing the effects of fabrication details on the mechanical properties and failure modes of woven composites of modern armor materials. By coupling it with PARADYN, a parallel explicit Lagrangian finite element code, within the message passing interface (MPI) scheme of PARADYN, a scalable local-global analysis model was created for conducting impact analyses of woven armor composites. Results are presented to demonstrate: 1. the verification of the RVE-TFA-PARADYN coupling, and 2. the scalability of the coupled model.

Keywords: 3-D woven composite, scalable computing, impact modleing

1 Introduction

Woven composites come in a variety of weaves, orthogonal, 2-dimensional, 3-dimensional, stitched, etc. They come with different fibers: glass, Kevlar, or carbon, and with different matrices. In military armor applications, their use comes from their superior personnel and structural protection from impacts. Since these composites can be made in a variety of weaves, braids, fibers and matrices, to effectively use these materials in short duration impact applications, one should be able to relate the weave construction details to the overall structural response. To achieve this, traditional finite element codes, which are essentially structural response providers, must be coupled with traditional composite micromechanics codes, which link the composite constituents' properties and local responses to the global composite properties; While this is being done, it is also important to relate the local failure modes at the fiber, matrix and weave level to the progression of damage observed at the global level.

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Weaving methods of fabric composites naturally give raise to repeating periodic local structures. The periodicity is apparent when a 3-D braid is built from several warp and weft layers and repeating in the third thickness direction. In contrast, a 2-D weave is made as a laminate of several layers, each layer made from two plane weaves, one each in warp and weft directions.

Dvorak (1992) described a modeling procedure using the TFA for Inelastic Composite Materials, and later Dvorak, Bahei-El-Din, and Wafa (1994) provided an implementation scheme of the TFA. Dvorak and Zhang (2001) used the TFA to analysis damage evolution in Composite Materials. Bahei-El-Din, Rajendran, and Zikry (2003) extended the TFA analysis to the study of plate impact problems of 3-D woven composites by considering a full complement of damage modes including matrix and fiber cracking, fiber sliding, interface failure and debonding.

When used in global impact analyses with explicit time integrations schemes, TFA analyses are conducted at each and every time step for the selected global finite elements. Since there can be many time steps in a global integration scheme, and since an RVE can contain many number of elements, depending on the details of a weave, the attendant RVE computations can be time consuming. Thus scalable computational approaches are needed to use the computationally intensive RVE-TFA.

With the objective of availing the RVE-TFA based damage propagation analysis to full 3-dimensional analyses of woven armor composite impacts, this paper presents results from an effort to link the serial

Proceedings of the 2004 International Conference on Computational & Experimental Engineering & Science 26-29 July, 2004, Madeira, Portugal

code used by Bahei-El-Din, Rajendran, and Zikry (2003) that generated the TFA coefficients as input to describe the material response provider to PARADYN, a general purpose explicit dynamics Lagrangian code. PARADYN is a parallel version of the Lawrence Livermore National Laboratory (LLNL)'s serial DYNA3D code. It is a natural choice for the present purpose because of it's large number of material models, contact algorithms, element types, etc. The linkage is done with the aid of domain decomposition and Message Passing Interface (MPI).

Since PARADYN is scalable, it already has its computational logic and data structures set for tackling its parallel computations. Even though, the code has facilities to add user defined materials and elements, the present RVE-TFA is neither a new material nor an element. Since potentially large RVE meshes can be considered requiring the storage of large amounts of RVE element specific material properties, stresses and strains data, using PARADYN data arrays for storing and retrieving such RVE-element data becomes intractable and potentially conflicting to the PARADYN scalability operations. To alleviate this situation, external processor specific files were used for writing the global elements' data and their respective RVE-elements' data. This enabled the RVE-TFA coupling without disturbing PARADYN code's MPI and domain decomposition based scalability operations.
To enable access to the RVE-TFA, a reference is provided to it as a Material Type 3 sub-option in PARADYN. This reference is completely arbitrary and could be placed even without getting into any material level subroutines. The data exchange between the codes occurs through external processor specific files. Thus with this interface, a dual level finite element modeling capability is added to the PARADYN code.

The outline of this paper is as follows. Section 2 presents the RVE-TFA equations for local stress representation. Section 3 presents the RVE-TFA approach for modeling the various damage mechanisms and damage progression specific to woven composites. Section 4 presents the details of the RVE-TFA coupling to PARADYN, and guide lines for its use. Section 5 presents verification, scalability and application of the coupled codes.

2. RVE-TFA Equations for Local Stresses

Figures 1 and 2 show, typical RVE's that can be used for modeling 3-D braids and 2-D weaves, respectively. Since gradual undulations are present in 2-D weaves, an RVE representing a 2-D weave can require a larger number of elements. Overall dimensions of these RVE's are neither arbitrary nor scalable; they are to be fixed based on the dimensions apparent in a weave's micrograph. While an RVE mesh density can be arbitrary, enough RVE sub-volumes are to be available such that each sub-volume belongs to a distinct phase: fiber bundle, matrix, or interface.

RVE-TFA rests on the fact that an RVE can be used to model the point-wise variation of stress (or strain) fields in a composite as sums of elastic stresses that are computed directly from the applied overall loads and some self-equilibrating local stress fields, i.e. which are significant within the RVE. Each of the self equilibrating RVE stress fields can be associated with an on-going damage progression within the RVE; the magnitude of each field can be determined to keep the stresses at levels as required by the damage criterion; and the effect of keeping some local RVE stresses at damage levels has to be balanced out by adjusting the local stress field to restore local equilibrium. The TFA, or the transformation field analysis, refers to the last step of local RVE stress adjustment.

A brief summary of the relevant equations of TFA is presented below. This is done using a notation of boldface lower case letters for representing the (6x1) stress/strain vectors, and boldface upper case letters for representing the corresponding stiffness/compliance matrices. The global stresses/strains, at an (integration) point where an RVE is called, are weighted volume sum of local sub-volume stresses/strains:

$$\overline{\sigma} = \sum_{r=1}^{Q} c_r \sigma_r \qquad \overline{\varepsilon} = \sum_{r=1}^{Q} c_r \varepsilon_r \qquad (1)$$

where, $\overline{\sigma}$ and $\overline{\varepsilon}$ are the global stress and strain, σ_r and ε_r the sub-volume stress and strain, Q the number of sub-volumes, c_r the sub-volume fractions.

The local sub-volumes are assumed to undergo elastic deformation. Deviations from this mode of deformation for accounting the effects of temperature, shape, inclusions, plasticity, and damage are treated by adding transformation fields. Symbolically, the local stresses/strains are expressed as follows:

$$\sigma_r = \mathbf{L}_r \varepsilon_r + \lambda_r, \quad \varepsilon_r = \mathbf{M}_r \sigma_r + \mu_r \qquad (2)$$

where, $\mathbf{L}_r$ and $\mathbf{M}_r = \mathbf{L}_r^{-1}$ are elastic stiffness and compliance, μ_r and $\lambda_r = -\mathbf{L}_r \mu_r$ are transformation strain and stress.

A part of the local sub-volume stresses/strains can be related to the global applied loads following the treatment of elastic composite aggregates by Hill (1963, 1965), the rest to a superposition of all the transformation fields originating in all local sub-volumes (within the RVE), Dvorak (1992) as

$$\varepsilon_r = \mathbf{A}_r \bar{\varepsilon} + \sum_{s=1}^{Q} \mathbf{D}_{rs} \mu_s,$$

$$\sigma_r = \mathbf{B}_r \bar{\sigma} + \sum_{s=1}^{Q} \mathbf{F}_{rs} \lambda_s, \; r = 1, 2,,,,,Q, \quad (3)$$

where, $\mathbf{A}_r$ and $\mathbf{B}_r$ are stress/strain concentration factors, $\mathbf{D}_{rs}$ and $\mathbf{F}_{rs}$ are transformation influence factors for the r^{th} local sub-volume. All these factors depend upon the RVE local geometry and properties of the local phases and can be determined from an elastic analysis of the RVE mesh.

The concentration factors, $\mathbf{A}_r$ and $\mathbf{B}_r$, are computed as statically equivalent to the global stresses available on the RVE. For example, the k^{th} column, k=1,2,,,6, of the stress concentration factor, $\mathbf{B}_r$, r = 1, 2,,,Q, is computed by giving a unit value to the k^{th} stress component and 0 to the rest of the 6x1 overall stress vector, $\bar{\sigma}$. This is done in the usual finite element sense by assuming a linearly varying local displacement field in the RVE, and by securing the RVE against rigid body deformation, (Dvorak and Teply, 1985).

A similar procedure is also used for computing the transformation influence factors by realizing that a k^{th} column, k=1,2,,,,6, of $\mathbf{F}_{rs}$, r,s=1,2,,,,Q, is a result of application of a unit stress, $\lambda_k = 1$, in the sub-volume V_s.

A total of 6Q RVE finite element solutions are required to completely evaluate the transformation factors. Since the RVE stiffness matrix remains the same, the only variants are the effective loads on the right hand side. The factors can be evaluated up front and made available to the RVE-TFA-PARADYN analyses.

Now the equations for computing the overall response in terms of local stresses/strains will be presented. Following Equation (1), these may be symbolically represented as

$$\bar{\sigma} = \bar{\mathbf{L}} \bar{\varepsilon} + \bar{\lambda}, \quad \bar{\varepsilon} = \bar{\mathbf{M}} \bar{\sigma} + \bar{\mu} \qquad (4)$$

where, $\bar{\mathbf{L}}$ and $\bar{\mathbf{M}} = \bar{\mathbf{L}}^{-1}$ are overall elastic stiffness and flexibility matrices. The overall transformation fields are related by

$$\bar{\lambda} = -\bar{\mathbf{L}} \bar{\mu}. \qquad (5)$$

By substituting the results of Equations (2) and (5) into Equation (1), the overall elastic stiffness and flexibility matrices can be evaluated as

$$\bar{\mathbf{L}} = \sum_{r=1}^{Q} c_r \mathbf{L}_r \mathbf{A}_r, \quad \bar{\mathbf{M}} = \sum_{r=1}^{Q} c_r \mathbf{M}_r \mathbf{B}_r \qquad (6)$$

The overall transformation fields also can be computed in a similar manner, (Levin, 1967, Dvorak, 1992), as

$$\bar{\lambda} = \sum_{r=1}^{Q} c_r \mathbf{A}_r^T \lambda_r, \quad \bar{\mu} = \sum_{r=1}^{Q} c_r \mathbf{B}_r^T \mu_r. \qquad (7)$$

3 RVE-TFA coupling to PARADYN

PARADYN is a general purpose explicit Lagrangian dynamics code with a capability for defining multiple element types and material types. The coupling is established such that each element of a global finite element model that is tabbed for detailed 3-d woven fabric analysis is made to call the RVE-TFA model to sample the local behavior and build the element global stresses from the constituent local stresses.

3.1 Guide lines for using the Model

The RVE-TFA analysis can be invoked as a material sub-option by specifying a Type 3 material and a non-zero number in the 5th data on the 8th material card. This material option describes a non-linear elastic-plastic response with kinematic and/or isotropic hardening. When the RVE-TFA analysis is specified for a material, a part of the input data needed for setting up the PARADYN's initial time step computations, i.e. the composite's overall material density, modulus and Poisson ratio, are read through the corresponding PARADYN material input data. The remaining data as well as the RVE mesh are read from additional input files: 1. RVE mesh comprising the usual nodes, elements and phases' material properties, and 2. stress and strain concentration factors, $\mathbf{A}_r$ and $\mathbf{B}_r$, and the transformation influence factors, $\mathbf{D}_{rs}$ and $\mathbf{F}_{rs}$ of Equation (3).

All this information is supplied to the RVE-TFA-PARADYN executable along with a domain decomposition part file. In fact this information is supplied through several separate files with specific names as follows: 1. "3drveprop" for the mesh definition and material properties, 2. "strscf" for the stress concentration factors, 3. "strncf" for the strain concentration factors, 4. "strsif" for the transformation influence factors, and 5. "umatin" for the phases' material properties.

3.2 Details of the Data Exchange

While PARADYN focuses on global computations such as the aggregation of nodal forces, solution of the equations of motion, updating global nodal positions, enforcing contact, etc., the RVE-TFA code focuses on the RVE calculations which typically involve evaluating the damage progression. For the respective codes to do their parts of computation, it is necessary that the relevant data be exchanged between them for each time step and for each global element identified for RVE-TFA computations. In the present work, the data exchange involved two parts as follows:

1. From PARADYN, at the beginning of each time step and for the identified global elements, the following data is written to external processor specific data files for read access to the RVE-TFA code: current time step, current global strain increments, global strains from previous time step, global stresses stresses from previous time step, and effective plastic strain from previous time step

2. After reading the PARADYN written data files, RVE-TFA code computes and writes the following data to external processor specific data files for read access to PARADYN: Effective density, Effective bulk modulus, Effective shear modulus, Computed current global stresses for the element, and Computed current effective plastic strain for the element

While PARADYN's native arrays are used for tracking global-stresses, global-strains, effective properties (density, bulk modulus, shear strain), and effective plastic strain, no such native arrays are used for the RVE element quantities. Instead these too are written to, and read from, processor specific files during each time step and updated during every time step. As opposed to the global-stresses of the global elements, the stored values of these responses reflect the accurate stress distribution within the RVE elements. During a PARADYN run, or after the run is complete, the processor specific files can be visualized independently for observing the local stress and deformation development.

4 Results and Discussions

The following numerical analyses are conducted for demonstrating the usefulness of the RV-TFA-PARADYN coupling for modeling 3-D woven composites. Scalability of the coupling was investigated on the ARL's SGI o3k machines.

4.1 An application of the RV-TFA-PARADYN coupling

For demonstrating the usefulness of the model coupling, the impact of a 5 mm thick steel plate a 25 mm thick 3-D woven, T300 carbon/epoxy composite was considered at a velocity of 200 m/s. Since the thickness of the target plate is small compared to its planer dimensions, a uni-axial strain condition is assumed in the target plate thickness direction. Referring to a composite micrograph, Figure 1, a 0.8 mm thickness is deemed necessary for using a 3-D woven fabric's version of the RVE mesh of type shown in Figure 1.

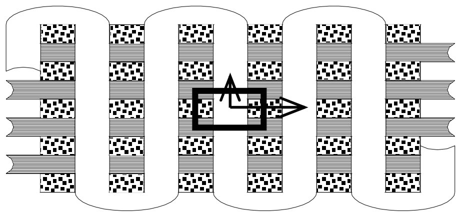

Figure 1. 3-D woven fabric's version of the RVE mesh

Accordingly, a global finite element mesh idealization with 40 elements was used, as shown in Figure 2. Each of the target plate global elements was modeled with 125 element RVE meshes.

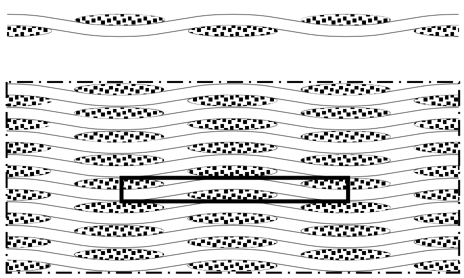

Figure 2. Finite Eleemnt Mesh for a 3-D Woven Composite

The result for the overall normal stress in thickness direction for the third global element from the impact surface was presented in Figure 3 for different impact velocities. For impact velocities less than 275 m/s, there is no permanent damage and the response is elastic. For larger velocities, the matrix ruptures leading to total composite failure.

The stress transient was compared with a result obtained from a serial run from, Bahei-El-Din, et al,

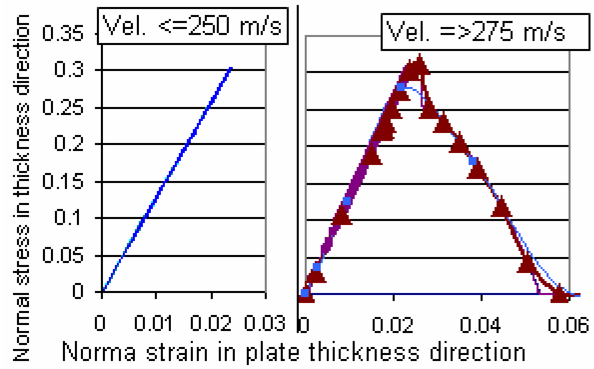

Figure 3. Overall stress vs. strain in the 3rd element from the impact surface

(2003). The on-set of the stress raise, stress magnitude, stress reversal and attenuation all agree with the result from the serial run. This was taken to verify the RVE-TFA's coupling with PARADYN. The noted deviation between the two results during

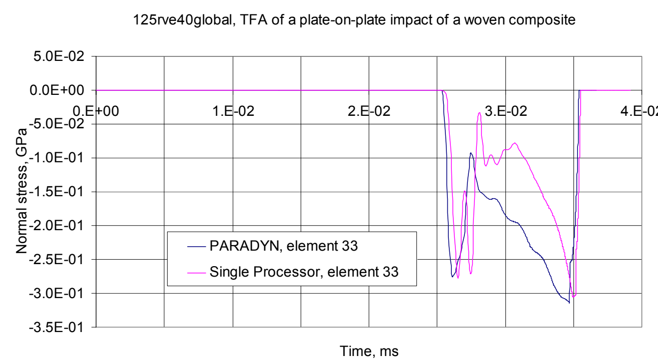

Figure 4. A comparison between results (normal stress for element #33) obtained from the single processor and PARADYN multiple processor runs.

the time between the stress peak and complete decay were thought to be attributable to the treatment of contact in the two runs.

Also the by-product of this coupled analysis are the detailed histories of the stresses in the 3D woven composite's constituents, different damage modes, and their progression as computed in each of the RVE meshes and their local elements at each and every time step. But to indicate the type of the stress-strain and damage information that can be obtained, the overall thickness stress vs. thickness strain for the third element under the impact surface was presented in Figure 4. This figure clearly shows an unloading that is different from the loading. The RVE results indicated an interface failure.

4.2 Scalability of the Results

As explained in Section 3.2, due consideration is given to the fact that PARDYN is a parallel code while coupling it to the RVE-TFA code. The coupling was done by keeping a global element's local computations local to the processor on which a global element resides. This meant that information such as local element stresses, strains and mechanical properties, stress and strain concentration factors, and transformation factors needed in the RVE computations are kept local and not passed into global data structures nor across processors. This meant that a global element's local stresses, strains and mechanical properties are needed to be written to, and read from, processor specific files in between time steps. To underscore the fact that the penalty associated with this approach is small, results from a limited scalability study are presented in this section.

No. of Processors	Wall Clock Time (sec)
2	102616
4	60543
8	38083
16	28546
32	26898

Table 1. Wall Clock Times for Scalability Study

The plate-on-plate impact problem of the previous section, with 40 global elements and 125 element RVE mesh, is used for this purpose. Runs with 2, 4, 8, 16 and 32 processors were made on zornig.arl.hpc.mil, an ARL MSRC's SGI computer. The wall clock times are presented in Table 1. An average 30% reduction in wall clock time was noted for each doubling of the number of the processors. Al though, this scalability is less than linear, the reductions in wall clock times from 28.5 hours with 2 processors to 7.9 hours with 16 processors is significant because such reductions allow the study of damage propagation in 3-D woven composites.

5 Future Work and Conclusions

3-D woven fabrics are used in the US Army's advanced structures and armor materials. Transformation field theories such as the RVE-TFA model described in this paper are being developed to model the effect of the fabric constituents on global material and structural responses. With the present coupling of the RVE based TFA analysis in PARADYN, many in-situ material damage progressions can be studied under diverse global impact conditions. The brief example application presented here demonstrated this. A transformation damage field analysis capability is added to PARADYN in a scalable manner. Local stress vs. strain histories in fabric constituents are produced together with damage progression because of this linkage under over all impact situations.

In future, the following extensions to this work will be considered: 1. using PARADYN's diverse material library to model the different phase materials, 2. modifying the RVE-TFA code and its data structures for additional parallelization to reduce the computation times, 3. modifying the RVE-TFA model to include an equation of state, and 4.extending the application range to include complex 2-D woven fabrics and diverse global applications

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