COVER SHEET

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Title: **Benchmarking of computational models for NDE and SHM of composites**

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ABSTRACT

Ultrasonic wave phenomena constitute the leading physical mechanism for non-destructive evaluation (NDE) and structural health monitoring (SHM) of solid composite materials such as carbon-fiber-reinforced polymer (CFRP) laminates. Computational models of ultrasonic guided-wave excitation, propagation, scattering, and detection in quasi-isotropic laminates can be extremely valuable in designing practically realizable NDE and SHM hardware and software with desired accuracy, reliability, efficiency, and coverage. This paper presents comparisons of guided-wave simulations for CFRP composites implemented using three different simulation codes: two commercial finite-element analysis packages, COMSOL and ABAQUS, and a custom code implementing the Elastodynamic Finite Integration Technique (EFIT). Comparisons are also made to experimental laser Doppler vibrometry data and theoretical dispersion curves.

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INTRODUCTION

The aerospace industry has seen an increased use of composite materials in recent decades, since composites can enable lightweight advanced aircraft and spacecraft designs. However, the current timeline for developing and certifying composite structures for use by industry and government can take over a decade [1]. NASA's Advanced Composites Project has the goal of reducing the timeline for certification of composite materials and structures [2]. Nondestructive inspection of composite materials for the detection and quantification of defects/damage is of key importance for certifying composite parts and ensuring the safety of aerospace vehicles.

Ultrasonic wave phenomena constitute the leading physical mechanism for non-destructive evaluation (NDE) and structural health monitoring (SHM) of solid composite materials such as carbon-fiber-reinforced polymer (CFRP) laminates. Computational models of ultrasonic wave propagation in CFRP laminates can allow for optimal designs of practically realizable NDE and SHM hardware (h/w) and software (s/w) with desired accuracy, reliability, efficiency, and coverage. Ultrasound models (analytical and numerical) solve the equations of motion with specified initial and boundary conditions. Numerical ultrasound simulations, such as finite element or finite integration methods, can incorporate appropriate material properties and morphologies of damage. However, several considerations enter into the practical implementation of a simulation code, thereby rendering each code "unique" in its details. These include

1. spatial scale of representation (fiber-, ply-, or plate-level specification of constitutive relationships, fine or coarse representation of faults);
2. spatio-temporal discretization of governing equations of motion and boundary conditions (finite-element *vs.* finite-difference, mesh density);
3. spatio-temporal duration of simulation (localized *vs.* extended response, space-time *vs.* wavenumber-frequency domain computation);
4. solver parameters (controlling stability, convergence, *etc.*).

The choices made in fixing these details for a particular problem must depend, to a large degree, on the experimental scenario that the numerical simulation is intended to represent. The chosen parameters essentially represent a trade-off between the accuracy and the stability of the code on the one hand, and its memory and runtime requirements on the other. While custom-developed codes can provide the user with significant flexibility in some of these details, taking proper advantage of such a capability requires a deep understanding of both the underlying physics and its numerical implementation on the part of the user. On the other hand, commercial codes tend to hard-wire some of these details in order to provide easy access to a larger community of users. Proper validation of simulation tools is required for both custom and commercial codes in order to ensure that the simulation setup and implementation are valid for the physical problem being studied.

In making an informed decision about the choice and the use of a computational modeling tool, the availability of benchmark problems with associated data sets and simulation studies is indispensable for composite material and structure designers, as well as for NDE and SHM h/w and s/w development communities. In this paper, we compare the performances of three different code bases on simulating ultrasonic guided waves in a pristine CFRP laminate as well as in laminates with delamination defects. The codes under consideration are two general-purpose finite-element

modeling codes, ABAQUS (from Dassault Systèmes) and COMSOL Multiphysics (from Comsol, Inc.), and a custom code implementation of the Elastodynamic Finite Integration Technique (EFIT) developed and used by the authors at NASA Langley Research Center. The pristine case simulation results are compared to experimental laser Doppler vibrometry data. For the delamination cases, the simulation results are compared to dispersion curve predictions of the dominant wavenumber occurring above the delamination region.

Memory and runtime requirements for each code are reported for each respective platform. Experimental data from this study will be made available to the research community in the hopes that additional codes may be run by other teams on the same problem in the future.

LABORATORY AND SIMULATION EXPERIMENTS

Experimental Data

In order to enable collection of experimental data for model validation and inter-comparisons, an eight-ply $[0/90]_{2s}$ IM7/8552 composite laminate was manufactured. The dimensions of the laminate were roughly 254 mm × 254 mm × 1 mm. Ultrasonic waves were excited with a 300-kHz, three-cycle, Hann-windowed sine wave injected by a contact transducer coupled to the back surface. Data were acquired using a 1D scanning laser Doppler vibrometer (LDV), Polytec OFV-505, measuring the out-of-plane velocity of the front surface.

Simulation Case Studies

Three simulation cases were implemented: 1) a pristine cross-ply laminate matching the specifications of the experimental artifact described above; 2) an identical laminate but containing a 15-mm square delamination beneath the 2nd ply layer; and 3) an identical laminate but containing a 15-mm square delamination beneath the 6th ply layer. For all three cases, the material parameters for IM7/8552 composite material were used in the simulations (see, *e.g.*, [3]). The simulation setup for the location of the excitation source (labeled "transducer") with respect to the location of the delamination is shown in Figure 1. This figure also shows how the ply depth of delamination is defined for the simulation results presented in the paper.

SIMULATION CODES

Some details are now given regarding the numerical simulation of guided-wave propagation in the experimental artifact described above. In all three codes, the excitation of waves was implemented as a displacement boundary condition over a 6-mm radius disk at the location of the transducer, having the same time profile as the actual electrical signal driving the piezo-electric crystal. While the dynamics of the crystal itself can, in principle, be modeled in codes like ABAQUS and COMSOL, this requires detailed technical specifications not readily available for most transducers. Other aspects of simulation differed slightly between codes, as indicated below.
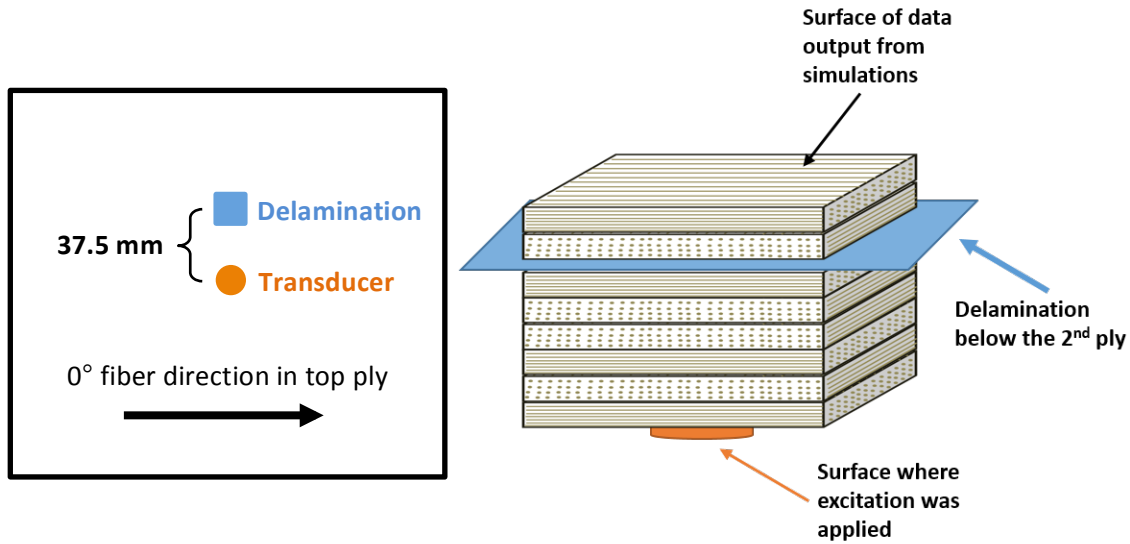
Figure 1. Diagram of simulation layout: (left) locations of the delamination and the transducer, and the fiber orientation in the top ply with respect to the propagation direction from the transducer to the delamination; (right) definition of delamination depth with respect to the excitation and the measurement surfaces.

Brief Description of ABAQUS

ABAQUS/Standard [4] is a versatile, flexible, and user-friendly finite-element analysis tool that features a dedicated implementation for layered solid composite materials. This makes it highly convenient for the modeling of guided-wave propagation in CFRP laminates. The ply thickness was taken to be 106.8 μm, and stress-free boundary conditions were employed at the edges of the computational domain. The delamination was implemented as two thin, detached Teflon inserts that were tied to the neighboring ply layers (*e.g.*, 2nd and 3rd). The 15-mm square delamination region was 13 μm thick, and rigidly tied to the rest of the laminate volume. The computational domain was meshed with hexahedral 8-point linear brick elements with reduced integration (C3D8R) and linear and quadratic geometric orders. In order to investigate the mesh sensitivity of the solver convergence, the mesh sizes were varied between 0.2-0.4 mm in the laminate and 0.1-0.25 mm within the delaminated volume, with 16 mesh elements through the plate thickness (*i.e.*, two per ply layer). The choice for simulation approach was ABAQUS/Implicit with dynamical time stepping seeded with an initial value of 1e-7 s.

Brief Description of COMSOL

COMSOL Multiphysics [5] is another user-friendly finite-element analysis platform that is ideally suited for the investigation of coupled multi-physics (electrical, mechanical, fluid, chemical) problems. Here, the ply thickness was again 106.8 μm, but an artificial exponentially absorbing boundary condition was implemented in order to keep the computational domain small (58 mm × 65 mm) without suffering from an early onset of boundary reflections. The delamination was implemented as a (zero-thickness) "thin elastic layer" – a built-in COMSOL option – with zero damping and

viscosity. A vanishing delamination thickness helps avoid excessively dense meshing around the defect. The damping parameters associated with this defect model implementation can be optimized to improve model fit to experimental data from delaminated panels, which were not available for this study. Several different meshing strategies and types were explored before converging on forming a tetrahedral surface mesh swept through the lamina layers, with two mesh layers per ply (*i.e.*, 53.4 μm depth resolution). The mesh sizes varied between 1.5-2 mm in the laminate and 0.25-0.7 mm in the delaminated volume. As is typical, the smaller the mesh resolution, the more accurate the frequency resolution and the smaller the time step needed to obtain a valid solution. The MUMPS parallelized direct solver used a maximum step size of 1e-7 s, and employed a generalized-α method with intermediate solver steps and a linear predictor.

Brief Description of EFIT

EFIT uses a mathematical approach that is similar to staggered-grid finite difference, and is an explicit time-domain method. Details regarding the EFIT approach and prior code validation work can be found in [3, 6]. The custom EFIT code used for the studies is parallelized to run efficiently on cluster and multi-core computing hardware. The EFIT code requires a spatial step size of approximately $\lambda_{min}/8$, where λ_{min} is the minimum wavelength in the simulation. For guided-wave simulations with delaminations, the wavelength above/below a delamination can be smaller than the wavelengths in the pristine regions of the simulated specimen. Therefore, expected wavelengths in the delamination region should be considered in order to capture the correct physics in the simulation. For the simulations presented in this paper, the EFIT spatial step size was 2.86e-5 m, and the time step was 2.17 ns. This spatial step size corresponds to 4 steps per ply layer. The EFIT simulation size for all cases in this paper was 90 mm × 60 mm × 0.92 mm, and the edges of the simulation domain were implemented as stress-free boundaries. For the delamination cases, the defect was implemented as a stress-free boundary condition in the delaminated region.

ULTRASOUND SIMULATION RESULTS

In this section, simulation results are compared with experimental data (for pristine case) and with dispersion-curve predictions (for delamination cases).

Pristine Case Results

For the pristine case, comparisons are made between experimental data and the results from the three simulation codes. Time-domain comparisons are shown in qualitative form in Figure 2 as snapshots in time of the out-of-plane velocity wavefield on the composite surface. Wavenumber-domain comparisons are made in Figure 3 as (k_x, k_y) plots at the excitation frequency (300 kHz). This approach for wavenumber-domain comparisons is discussed further in [3, 8]. Table I gives a quantitative comparison of the dominant wavenumber in directions parallel and perpendicular to the top-layer 0° fiber orientation (as indicated in Figure 1).
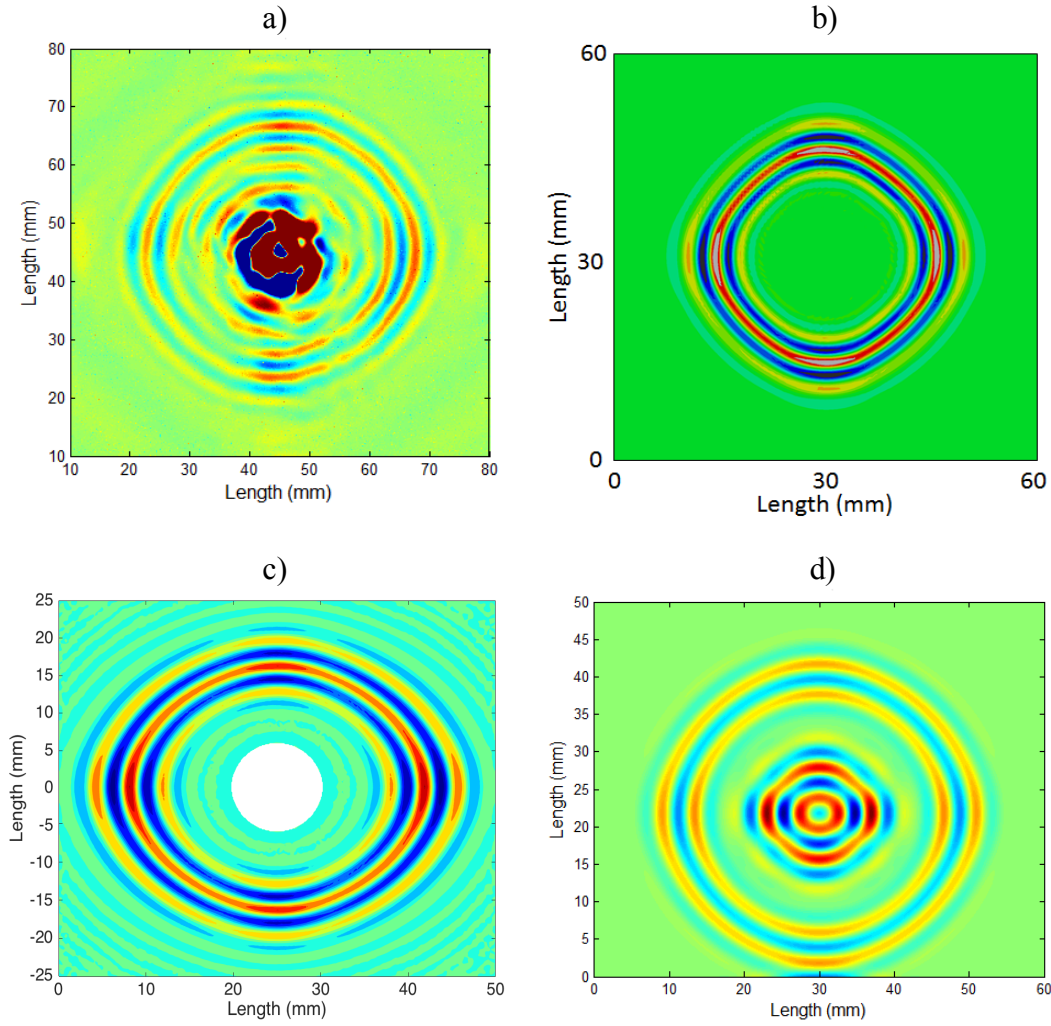
Figure 2. A snapshot in time, at approximately 1.30e-5 s after the initial excitation, showing the out-of-plane velocity on the surface of the pristine cross-ply composite from a) experimental data, b) ABAQUS, c) COMSOL, d) and EFIT. The white circle in the middle of c) roughly marks the location of the excitation boundary condition.

TABLE I. WAVENUMBERS, PRISTINE CASE

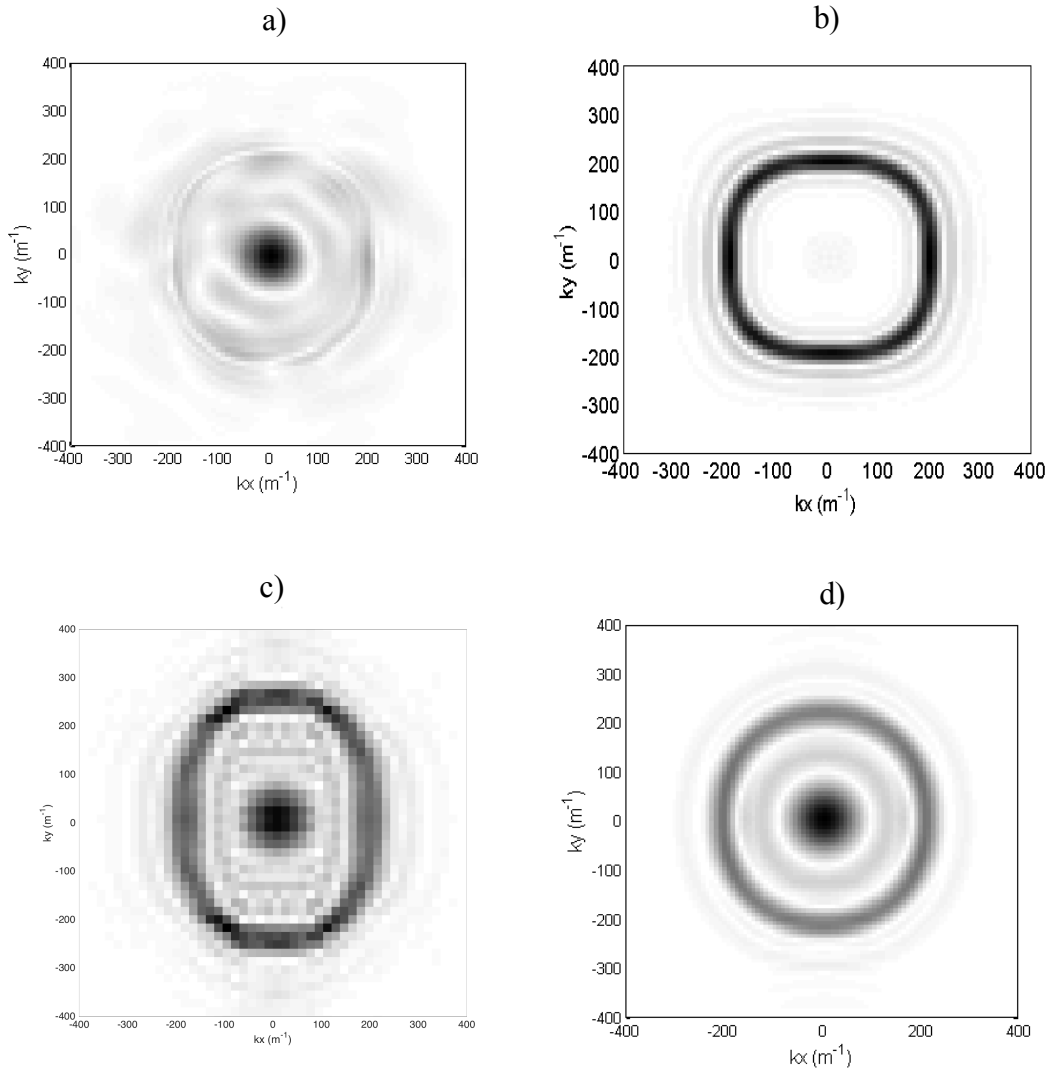| Direction	Wavenumber (m^{-1})			
	Experiment	ABAQUS	COMSOL	EFIT
∥ to 0° fiber orientation	200	190	250	209
⊥ to 0° fiber orientation	225	210	200	221

Figure 3. Pristine sample wavenumber plots at 300 kHz temporal-frequency slice from a) experimental data, b) ABAQUS, c) COMSOL, and d) EFIT.

Delamination Case Results

For the delamination cases, comparisons are made in time and in wavenumber domains between the three simulation codes, and wavenumber results calculated for the 15-mm square region above the delamination are compared to dispersion curves created using the DISPERSE software [7]. Comparisons of simulation results in both time domain and wavenumber domain are shown below in Figures 4 and 5 for case 1 (delamination beneath 2nd ply) and in Figures 6 and 7 for case 2 (delamination beneath 6th ply). The 3-D fast Fourier transform used to generate the wavenumber-domain plots was only applied to the wavefields above the region of delamination. Table II gives a quantitative comparison of the dominant wavenumber above the delamination region in the direction perpendicular to the top-layer 0° fiber orientation (as indicated in Figure 1).
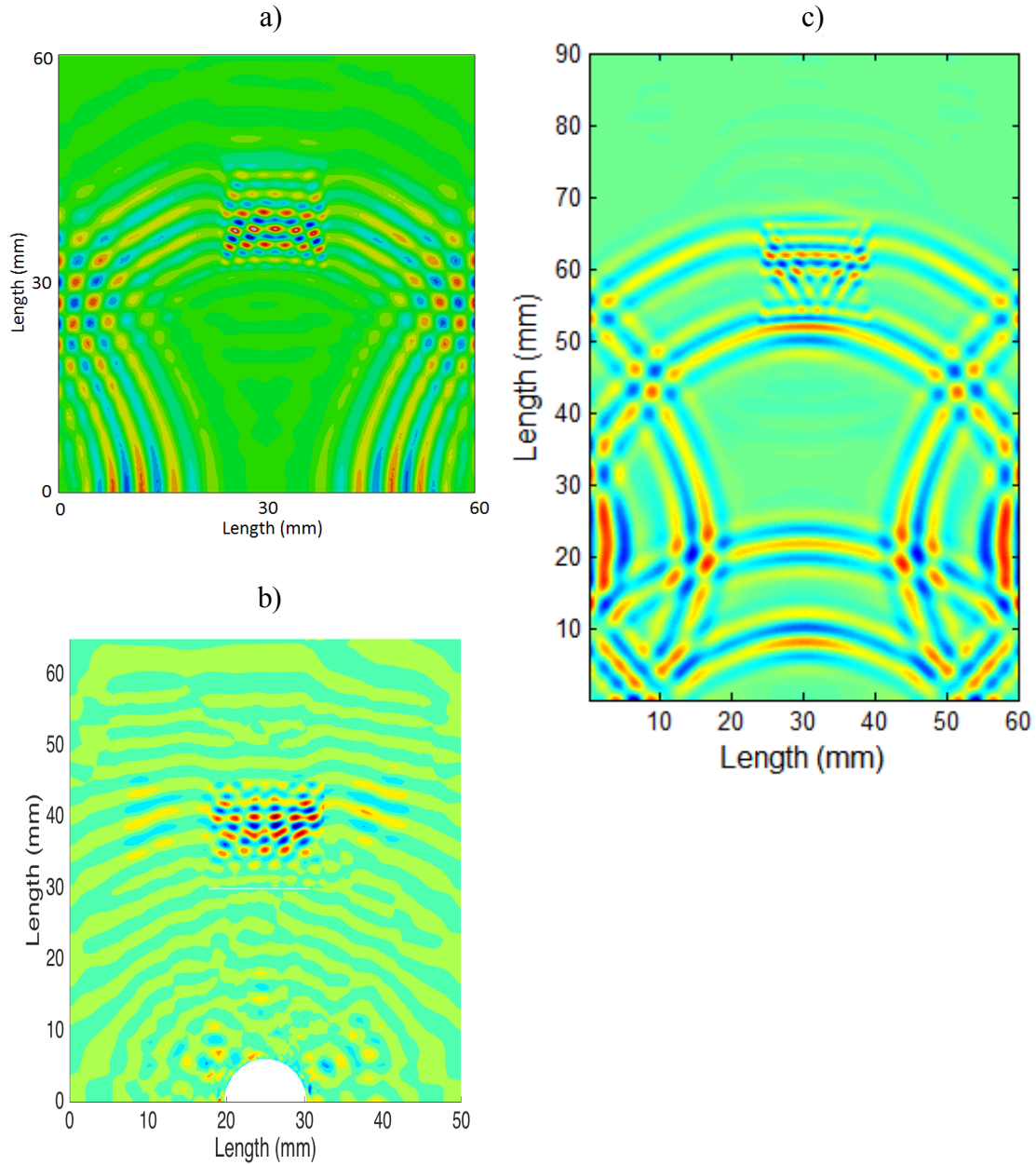
Figure 4. Snapshot, at 3e-5 s after start of excitation, of the out-of-plane velocity for the case of a delamination below the 2nd ply; a) ABAQUS, b) COMSOL, and c) EFIT.

TABLE II. WAVENUMBERS ⊥ to 0° FIBER ORIENTATION, DELAMINATION CASES

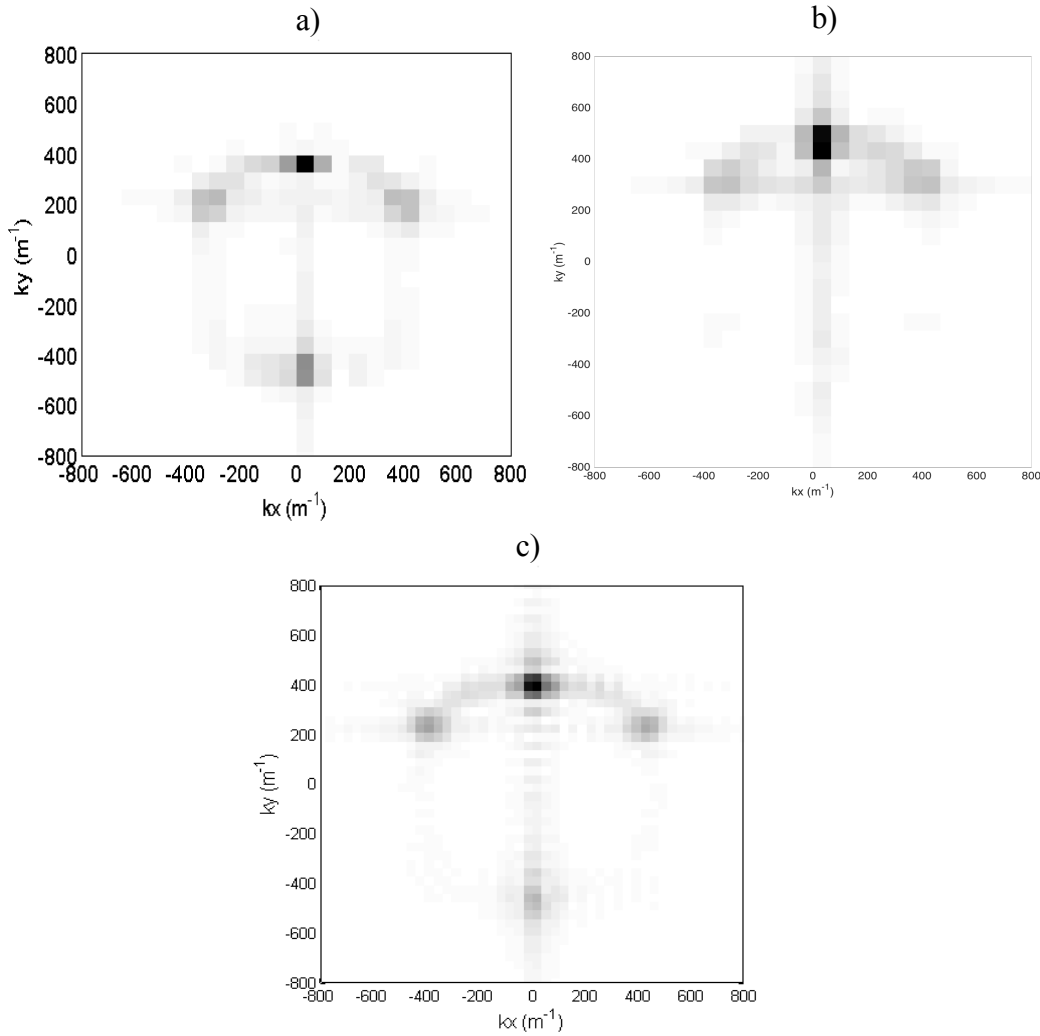| Delamination	Wavenumber (m^{-1})			
	DISPERSE	ABAQUS	COMSOL	EFIT
below 2nd ply	418	367	466	410
below 6th ply	275	233	300	273

Figure 5. Wavenumber-domain comparison for the 300 kHz frequency slice with delamination below 2nd ply; a) ABAQUS, b) COMSOL, and c) EFIT.

DISCUSSION OF RESULTS

Relative Accuracy

As can be seen from Table I, all three simulations match fairly well with experimental LDV data on the pristine specimen, with ABAQUS, COMSOL, and EFIT matching the data to within 5.8%, 5.6%, and 3.1%, respectively (averaged over two orthogonal directions). A slight edge for EFIT emerges for the delamination cases reported in Table II as compared with wavenumber predictions from theoretical dispersion curves calculated by DISPERSE. For case 1 (delamination below 2nd ply), ABAQUS, COMSOL, and EFIT match the predicted wavenumbers to within 12.2%, 11.5%, and 1.9%, respectively. For case 2 (delamination below 6th ply), ABAQUS, COMSOL, and EFIT match the predicted wavenumbers to within 15.3%, 9.1%, and 0.7%, respectively. The wavenumber plots for both cases show that the ultrasonic energy incident on the delamination is scattered predominantly in the forward direction.
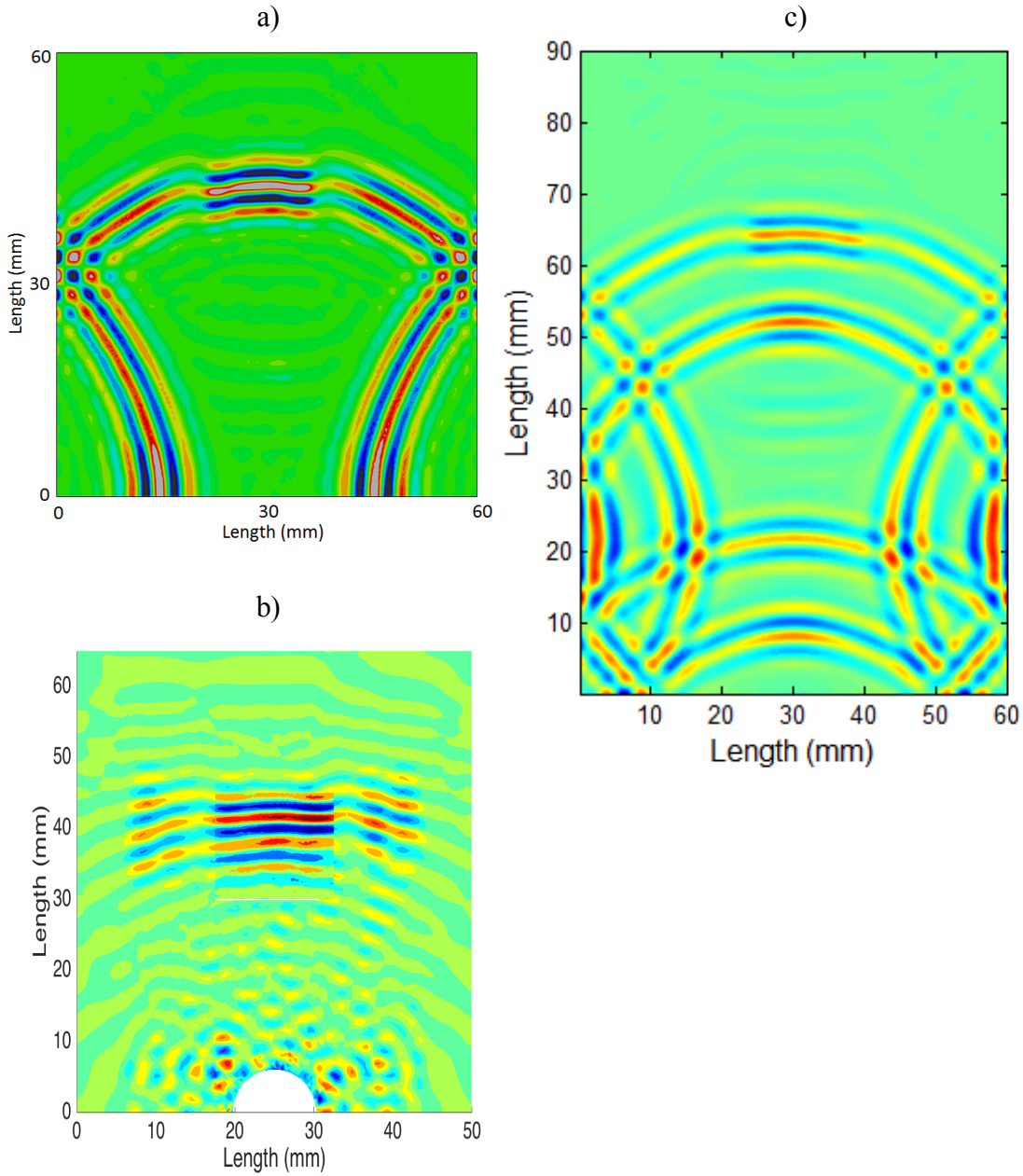
Figure 6. Snapshot, at 3e-5 s after start of excitation, of the out-of-plane velocity for the case of a delamination below the 6th ply; a) ABAQUS, b) COMSOL, and c) EFIT.

The simulated wavefields in Figures 4 and 6 demonstrate convincingly that shallower delaminations have a stronger effect on propagating waves, thus making their detection considerably easier, as would be expected intuitively. The absence of boundary reflections in COMSOL is noteworthy in comparison with ABAQUS and EFIT results, which is due to the different boundary conditions employed. The corresponding wavenumber patterns in Figures 5 and 7 further substantiate this observation. A useful conclusion here is that, when using an NDE tool such as the LDV, laminates should be inspected from both sides, if practically possible, in order to improve the probability of detection.
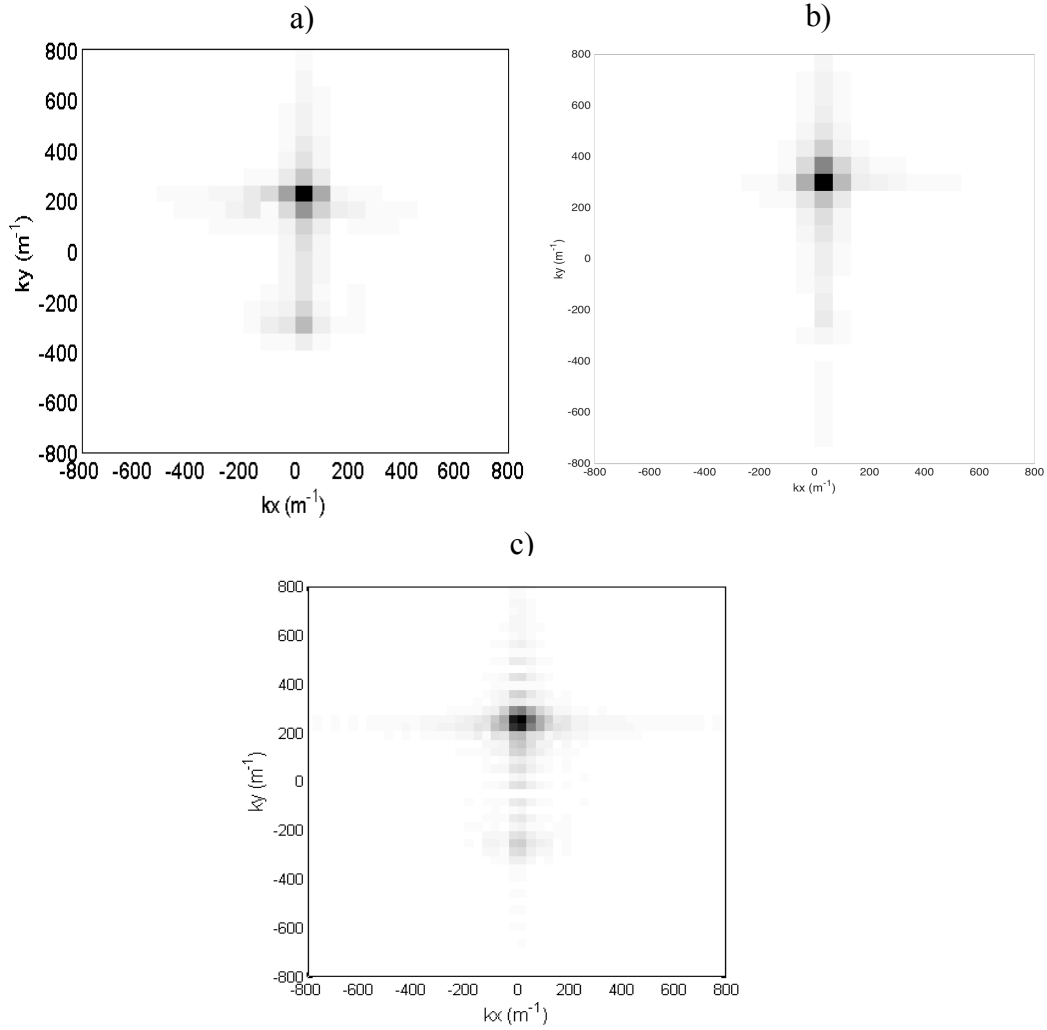
Figure 7. Wavenumber-domain comparison for the 300 kHz frequency slice with delamination below 6th ply; a) ABAQUS, b) COMSOL, and c) EFIT.

It is also illuminating to compare time-domain waveform propagation among the three codes. Figure 8 shows the spatial variation, up along the vertical midline of the pristine panel, of the normalized out-of-plane velocity, with the point $y = 0$ corresponding to the center of the transducer. ABAQUS, COMSOL, and EFIT results are displayed at time instants of 1e-5 s, 2e-5 s, and 3e-5 s. The fast (S0) and slow (A0) waves are both clearly visible, as well as an appreciable difference in the group velocities of the simulated wavepackets. A satisfactory explanation of this discrepancy requires a deeper understanding of the internal workings of each code, which will be reported on in a subsequent publication.

Computational Platforms and Requirements

A direct comparison between the computational resources required by the various simulation codes is difficult since they are parallelized differently, have different step-size requirements, and were run on different hardware. We therefore document the details of each code separately below.
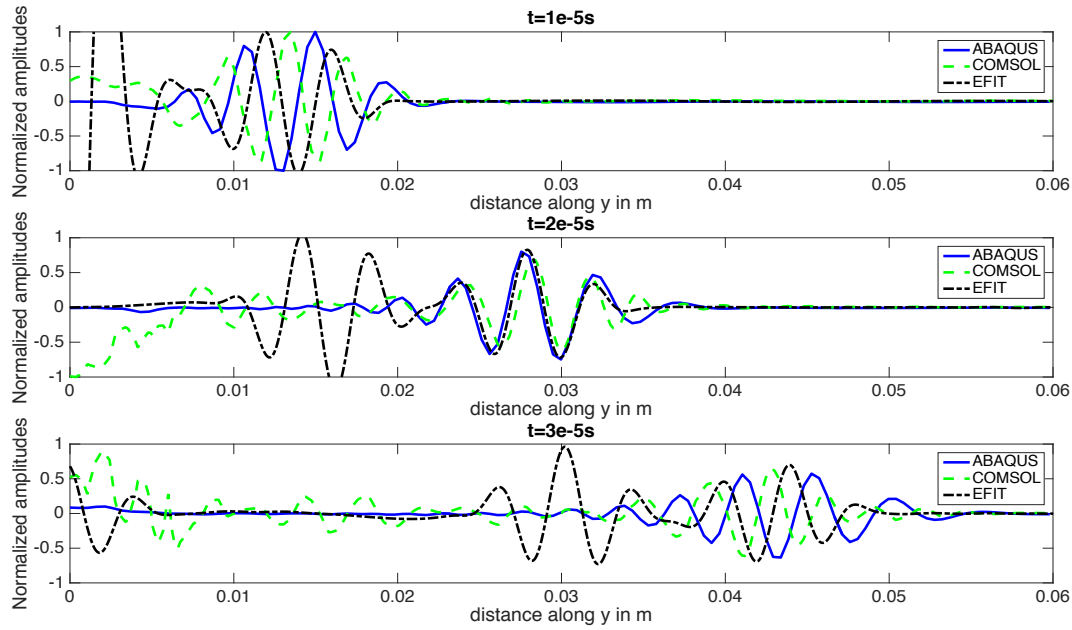
Figure 8. Time-domain comparison of normalized out-of-plane velocities at different time instants along the direction perpendicular to the top-ply 0° fiber orientation.

ABAQUS. These simulations were performed on two separate Linux Red Hat Dell workstations, one with 189.2 GB of RAM and 7 Intel Xenon processors W5590 running at 3.33 GHz, and the other with 441.8 GB of RAM and 16 Intel Xenon processors E5-2697 running at 2.7 GHz. The time step was dynamically adjusted between 0.5 to 4 times the seed value of 1.7e-5 s. The mesh size within the delamination region was kept at 0.2 mm, while in the rest of the laminate the mesh density was varied from 0.6 down to 0.2 mm. The corresponding numbers of degrees of freedom (DOF) varied between 1.4 and 4.44 M, requiring 30 to 60 GB of memory and taking anywhere from 15 to more than 40 hrs of CPU time, respectively, to complete a 30-μs simulation.

COMSOL. The CPU hours are reported for two different machines. The Intel-based platform is a Dell Precision T7600 workstation with 512 GB of RAM and with 16 Intel Xeon CPU E5-2687W processors running at 3.10 GHz with 20 MB cache, running Red Hat Enterprise Linux Kernel 2.6.32-642.el6.x86_64 (Red Hat 4.4.7-17). The AMD workstation used a Super-micro motherboard with 32 AMD Opteron 6380 processors running at 2.5 GHz with 2 MB cache, with 1 TB of RAM and running Red Hat Enterprise Linux Kernel 3.10.94-1.el6.elrepo.x86_64 (Red Hat 4.4.7-16). The AMD machine was newer and had more CPUs and more memory, but typically ran half as fast as the Intel-based machine running the same COMSOL models and same version of COMSOL. We attribute this to sub-optimal library optimization, as well as to the fact that AMD processor pairs share a floating-point unit – a big disadvantage for floating-point-heavy utilization.

The time step was fixed at 1.7e-5 s for 30-µs simulations. The mesh elements within the laminate varied between 1.5 to 2 mm, while those in the delamination region were between 0.25 to 0.5 mm (fine) or 0.5 to 0.7 mm (coarse). This resulted in DOFs of 807 K (38 GB) and 1.575 M (59 GB) for coarse and fine meshes, respectively. CPU hours for the coarse mesh were 29 and 60.5 for Intel and AMD, respectively, and 80.65 and 168.25 hrs for the fine mesh.

EFIT. The EFIT simulations were run on 36 CPU cores (Intel Xeon E5-4650 2.4 GHz). These simulations had approximately 211 M grid points (1.9 billion DOFs) with a spatial step size of 2.86e-5 m throughout the simulation. The time step was set to 2.17 ns, as required by the EFIT approach [3]. A single simulation took 60 hours to run to 40 µs (~18400 time steps). A single simulation required 105 GB of memory.

CONCLUSION

In conclusion, all three codes under study – ABAQUS, COMSOL, and EFIT – are capable of capturing the essential physics involved in the propagation of guided waves in pristine CFRP laminates and the scattering of such waves by delamination defects, despite the different approaches adopted within each code. They each offer a unique set of features and capabilities, which may make them more or less suitable for a given problem. As evidenced by the superior accuracy of EFIT over ABAQUS and COMSOL in the delamination cases, a denser mesh and time stepping do pay off, but come at the expense of additional computational resources (memory and runtime).

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