Enriched Numerical Method for Wave Propagation and Assessing Material Damage

Using Nonlinear Acoustics

by

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Thesis submitted in partial fulfillment of the requirements
for the degree of Doctor of Philosophy in Civil Engineering
in the Graduate College of the
University of Illinois at Chicago, 2018

Chicago, Illinois

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To my amazing mom and dad,

Ashraf Foroughi Shafiei and Khosro Kamali Zououzi,

Without whom none of these would exist. Every word of this dissertation, every step of the Ph.D journey would not be possible without echoes of my dad’s Tar in my ears and the vivid colors of my mom’s paintings in my eyes.

Me having an engineering doctorate degree in my hands, started when my 20 year old dad started his own undergraduate degree in Mechanical Engineering in the University of Tehran, my most favorite place on earth, and it continued to shape by watching amazing and powerful women in my life like my mom and both my grandmothers, Tayebeh and Roghayeh.

And to my younger brothers Sahand and Nima, who are the essence of my life, and who had to endure being away from their amazing sister so that she can do her Ph.D. and were not secretly happy that their sister was not there to boss them around.

I stepped into the Ph.D program, leaving all my family and friends, my childhood memories and all the other big and small things I may never be part of again. I’m quoting my favorite dialogue from the movie Brooklyn:

”you’ll feel so homesick that you’ll want to die, and there’s nothing you can do about it apart from endure it. But you will, and it won’t kill you. And one day the sun will come out - you might not even notice straight away, it’ll be that faint. And then you’ll catch yourself thinking
about something or someone who has no connection with the past. Someone who’s only yours. And you’ll realize... that this is where your life is.”

Would I ever be strong enough to endure the hardship of being thousands of miles away from my family without my amazing and beautiful people in Chicago, who are my friends and my family.

I’m indebted to my friend, my mentor and my long-sought-after sister Pantea Vaziri who took me under her wing, kept me sound and sane and helped me find the sunlight in my most cloudy days. I can’t imagine myself and my life here in Chicago without her and my beautiful, smart and amazing Manisha J. Mugunthan!

I’m thankful to my best friend and my partner in crime, Niloofar Tehrani, another fellow Ph.D. from UIC for stalking me on Facebook for months until I accepted to be real-world friends with her, and was able to tease her in the real world. She stayed by my side and was there for me in all ups and downs of Ph.D student life. Together we were able to found the most amazing part of my UIC experience, Grad SWE UIC.

I’m thankful to my twin-sister-friend Mahsa Modiri who is a reminiscent of an 18 year old Negar. She is a non-separable part of my life since 2005 and gladly we were never apart more than a two hours drive ever since.

I’m thankful for the friendship of my girls, Sara Shahi, Elham Kazemi, Maryam Mortazavi, Maryam Nazari, Selin Yaman, Hilal Saglam and Roya Zanjani.
I’m thankful for the friendship of all the amazing SWE UIC crew and special thanks to Elsa Soto for all the help and support for Grad SWE UIC.

And last but not least, I’m thankful to my lab mates and friends Ashkan Mahdavi, Thanakorn Siriaksorn, and Muhammed Mujtaba Atif for all their help and support in my PhD journey.

Shout out to all the other Ph.D and M. Sc. Students in SEL 4462 for creating all the fun memories that I can talk about to my grand children.

As this journey ends, another begins and I can’t wait to enjoy post Ph.D. life among all my beloved friends and family, specially my new family at Skidmore, Owings & Merrill LLP.

And the rest is history.
Painting by Ashraf Foroughi Shafiei
ACKNOWLEDGMENTS

I can honestly express that my academic journey would not have been possible without the constant technical guidance, support and tremendous belief received by my Ph.D advisor Prof. Sheng-Wei Chi. I am deeply grateful for the continuous help and generous collaboration received which have helped me grow both on a personal and academic level. I would like to thank my committee members, Prof. Craig Foster, Prof. Didem Ozevin, Prof. Ernesto J. Indacochea and Prof. Gerard Awanou for providing their valuable time and through their presence.
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<td>FE</td>
<td>Finite Elements</td>
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<tr>
<td>UT</td>
<td>Ultrasonic Technique</td>
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<td>NLUT</td>
<td>Nonlinear Ultrasonic Technique</td>
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<tr>
<td>FFT</td>
<td>Fast Fourier Transform</td>
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<tr>
<td>WT</td>
<td>Wavelet Transform</td>
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<tr>
<td>HOH</td>
<td>Higher-order-harmonics</td>
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<td>RKPM</td>
<td>Reproducing Kernel Particle Method</td>
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<td>H-RKPM</td>
<td>Harmonic-Enriched Reproducing Kernel Particle Method</td>
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CHAPTER 1

INTRODUCTION

1.1 Motivation

In order to ensure built structures functionality and assess their remaining service life, it is essential to detect microstructural damages in structural elements. The use of ultrasonic testing in detecting damages in materials is well established. Linear ultrasonics techniques provide satisfactory detection capabilities for defects with a length scale much larger than the ultrasound wavelength. However, when the defect size is close to or smaller than the ultrasound wavelength, linear ultrasound technique is not applicable (1). Detecting large cracks, sometimes, is too late to prevent a catastrophic failure of a structure because the damage has developed enough to deteriorate the structure rapidly. Investigating damages in early stages, therefore, is of utmost benefit, but beyond the bounds of possibility for linear ultrasonics. Due to the limited capability of linear ultrasonics, nonlinear ultrasonic methods are used in order to detect smaller damage.

Under the nonlinear ultrasonics, the damage in the material alters the nonlinear material properties, which can be quantified by the phase changes or wave speed changes of the ultrasound waves. Acoustic nonlinearity parameter, is one of the most popular tools for measuring the material nonlinearity, which is proportional to the ratio of the second harmonic amplitude to the square of the first harmonic amplitude: \( \frac{A_2}{A_1^2} \) (2, 3). However, it is challenging to understand how the effects of various damage modes correlate with the changes of nonlinear material properties by merely using experimental techniques. The
numerical modeling, therefore, plays an important role for predicting and correlating the behavior of nonlinear ultrasound throughout a variety of damage conditions and offers a means to gain insight into the contribution of different damage modes such as microstructural evolution, meso-scale heterogeneity, geometrical variation, etc. and the ultrasound signal.

There are many cases where the initiation of macroscale damage in a structure is preceded by evolution of the microstructure of the material. Material heterogeneity, creep and fatigue are some of the forms of microstructural variation.

The ultrasound predicted in a heterogeneous medium is crucial due to many applications such as detecting damage in porous media, composites, granular material, or in diagnostic and therapeutic ultrasound (4). The heterogeneous components distort the wave resulting in changing the phase and generating higher order harmonics. There are many experimental studies showing the greater sensitivity of the third harmonic to the microstructural evolutions. When plastic strain is localized, the third harmonic ratio $\frac{A_3}{A_1}$ appears to increase with a greater value in comparison to the second harmonic. Moreover, further research shows that higher-order-harmonics are present when variations exist in any scale. Microscale variations (such as grain boundaries, dislocations), meso-scale variations (such as precipitates, intermetallics, etc) and macroscale variations (such as holes, welds) also contribute to higher order harmonic generations. However, their specific role in the nonlinearity of the material is still under investigation.

Numerical methods have been used for solving linear and nonlinear wave propagation problems in homogenous and heterogeneous solids for more than 50 years. In spite of great success of finite element method in solving boundary value problems, there has been growing interest in improving the method even further. Although considerable effort has been made to developing finite elements methods, the
currently available techniques become computationally less efficient as the problem requires smaller mesh size or complicated structures. The errors incorporated in wave propagation analyses using the piecewise polynomial approximations of standard Finite Element methods have been recognized and analyzed \(^5\) \(^6\). As far as time harmonic wave propagation problems are concerned, the fact that the accuracy of the numerical solution gets diminished rapidly with increasing the wave number is well understood \(^7\) \(^8\) \(^9\) \(^10\) \(^11\). Hence, to obtain valid and feasible solutions for problems with very short waves, very fine mesh needs to be maintained in the model, to such extent that the computational solution effort may be limiting. When dealing with wave propagation problems, numerical wave propagation velocity might not equate to the physical velocity, due to the numerical period elongation and amplitude decay \(^12\) leading to the dispersion and dissipation errors \(^12\) \(^13\) \(^14\) \(^15\) \(^16\) \(^17\) \(^18\) \(^19\) \(^20\) \(^21\).

As a wave travels, the dispersion and dissipation errors accumulate and the numerical solution becomes inaccurate. Therefore, whenever high-frequency components are present in the solution, significant errors are present in the numerical solution unless the mesh is fine enough to model the high-frequency wave. Although there are few numerical studies on nonlinear ultrasonics, a more advanced and accurate numerical modeling is required to overcome the accuracy and efficiency shortcomings in nonlinear ultrasonics problems, especially when harmonics higher than the second harmonic is needed to be captured. Accurately capturing higher harmonics requires an even smaller element size. As the dispersion accuracy is demanded, the element size in FE needs to be 20 times smaller than the wavelength of the harmonics \(^22\). This issue affects the computational efficiency and accuracy, which further
demonstrates the demand for a more efficient computational technique to solve nonlinear wave propagation problems.

To enhance computational efficiency while achieving solution accuracy for the prediction of high frequency responses, one approach is to use higher-order elements \((23)(24)(25)(26)(27)\). This method generally provides us with a more accurate solution; however, the computational cost increase may surpass the gain it may offer, often due to additional degrees of freedom added. Another approach is to introduce problem-specific enrichment functions as the basis function in the numerical method so that it can capture the higher-order-harmonics more effectively.

1.2 Objective

The objective of this research is divided into two main parts. The first part describes numerical simulation of nonlinear ultrasonic wave propagation with an intention to acquire deep understanding on how different-scale non-homogeneity sources can contribute to higher-order-harmonics. To do so gives us an insight when quantifying the nonlinearities or damage of the material and enables us to effectively mitigate the possibility of failure and anticipate the service life of a structure. The numerical results are verified with experimental testing. Since the NLUT relies on high frequency components in order to detect damages shorter than the linear UT wavelength, the second part of the dissertation deals with enhancing the existing numerical methods such that they are capable of solving the high frequency wave propagation problem more accurately and efficiently. Numerical results were validated with several benchmark problems and analytical predictions. Specific research development made are summarized as follows:
(1) Post processing techniques based on Fast Fourier Transform and Wavelet Transform are studied and advantages and disadvantages of each method is described. The accuracy of each method on calculating the nonlinearity parameter from an ultrasound signal is discussed. The influences of the sampling rate, frequency range and duration of the time domain response to the result of frequency spectrum in calculating the nonlinearity parameter were examined. Results show that wavelet transform has better resolution for extracting high order harmonics. All NLUT nonlinearity calculations in this thesis were conducted based on the Wavelet Transform post processing technique.

(2) The relationship between statistical variation of microstructure and the predicted ultrasound in the mesoscale model is studied. The study quantifies how the statistical variation in heterogeneity size, volume fraction, standard deviation, and distribution in microstructure affect the received ultrasound in the continuum level. The numerical results suggest that the third harmonic has greater sensitivity with regards to the random heterogeneity characteristics, which is supported by numerical studies in the literature.

(3) A thorough study has been done to investigate the contribution of different scales variations and heterogeneities on higher-order-harmonics. Numerical models representing micro-scale variations, mesoscale heterogeneities and macroscale variations are constructed and acoustic nonlinearity parameters are derived for each case. A broader understanding of the sources of higher-order-harmonics are obtained and the greater contribution of the third-order-harmonic when the above-mentioned variation exist is confirmed. The results are verified with NLUT experiments and XRD image processing.

(4) An enriched finite element method is employed to effectively obtain numerical solutions of nonlinear wave propagation problems. One-dimensional and two-dimensional benchmark problems
are verified. Three dimensional problems are approached similarly. The method merges the assets of finite element (FE) and spectral methods while conserving the core properties of FE. Additional degrees of freedom corresponding to higher harmonic terms are added to the nodes of standard FE elements. The essential boundary conditions in the enriched finite element method can be imposed by Nitsche’s method to further reduce the solution error. Efficiency and accuracy of the numerical method have been discussed. A User-defined element (UEL) and user-defined material (UMAT) are developed and incorporated in Abaqus to solve nonlinear wave propagation problems.

(5) A harmonic-enriched reproducing kernel particle method (RKPM) is developed with the aim of enhancing the accuracy of the high frequency wave propagation problems while increasing the computational efficiency even further. One-dimensional and two-dimensional problems are studied and the results are compared with FE, standard RKPM, enriched FE and analytical solutions. In this method, higher harmonic terms are inserted into the basis function, without adding degrees of freedom. Special consideration of the essential boundary conditions is required and as for the enriched FE, Nitsche’s method is employed to handle the essential boundary conditions imposition. Von Neumann analyses have been conducted to assess the dispersion and stability properties of the newly developed method.

The organization of the thesis is as follows. Chapter 2 will review the critical literature on Nonlinear ultrasonics and numerical methods to solve nonlinear wave propagation problems. The theory of nonlinear wave propagation will be described in Chapter 3. In Chapter 4, a review and comparative study of signal processing techniques is offered. Higher harmonics in nonlinear ultrasound testing and their relationship to microstructural evolution is discussed in Chapter 5. Numerical studies on the influence of different scale heterogeneities on higher order harmonics under plastic deformation is described
in Chapter 6. In Chapter 7, enriched finite element methods are applied to solve wave propagation problems. Chapter 8 describes the harmonic-enriched RKPM method for solving the wave propagation problems. Lastly, conclusions and future work will be discussed in Chapter 9.
CHAPTER 2

LITERATURE REVIEW

A literature review is presented here on the subjects of nonlinear ultrasonic wave propagation and numerical modeling. Since the objective of this study is more numerically oriented, the literature review therefore has an emphasis on the numerical aspects of nonlinear ultrasound testing. In Section 2.1, early studies of nonlinear ultrasonic testing and signal processing methods are reviewed. More enriched numerical techniques previously utilized are described. Based on these reviews, challenges to nonlinear wave propagation and multiscale study in heterogeneous media are summarized. Later, studies on numerical methods to solve wave propagation problems regarding ultrasound testing and developing correlation between damage and higher harmonics are reviewed. Enhanced numerical methods to solve for wave propagation problems and their challenges are reviewed next.

2.1 Nonlinear ultrasonic testing and signal processing

Theories of finite amplitude wave propagation dates back to the 18th and early 19th centuries by Euler, Poisson, and Lagrange (28). Investigation was continued in the 19th century by Earnshaw (29). In 1935 Thuras et al. (30) discussed harmonic generation phenomena in air. In the late 1950’s, interest in nonlinear acoustics began to increase. Krassilnikov et al. (31) published an experimental observation of the harmonics in a traveling wave of finite amplitude in 1957. Romanenko (32) performed experimental studies of finite amplitude spherical waves in 1959. Ryan et al. (33) measured harmonic content as a function of propagation distance in 1962. Studies of harmonic generation in solids began in the early
Breazeale and Thompson (2) and Hikata et al. (34) measured harmonic generation in aluminum. The development of nonlinear acoustics has been widely reviewed, for example by Bjørnoøø (28) and by Breazeale and Philip (35). Of particular importance was the discovery in the early 1970’s by Gits et al. (36) of the correlation of fatigue damage in aluminum with nonlinear distortion of ultrasonic waves.

Since then, Ultrasonic technique (UT) has been used as a nondestructive evaluation (NDE) technique that characterizes the material state the propagation of high frequency sound waves within the material and has been vastly employed to identify the presence of surface flaws such as cracks as well as internal flaws such as voids or inclusions in materials (37) (38). Although linear UT has many applications, it becomes considerably less accurate when the defect’s size is smaller than the ultrasound signal’s wavelength, which limits the capability of characterizing the microstructural defects, such as early stages of fatigue and creep damage. On the other hand, microstructural defects or heterogeneities scatter and distort the sound wave leads to further nonlinearity making the use of nonlinear UT inevitable (39), (40), (41). The material nonlinearity in the nonlinear wave propagation theory is assumed to be associated with the homogenized properties of microstructural defects or heterogeneities which can be determined by stress dependent ultrasonic wave speed known as acoustoelasticity (42), (43), (44), (45) or the detection of higher harmonics (46), (2), (47), (48).

When the fundamental wave mode propagates in a material, the interaction of the fundamental wave mode with microstructural damage generates higher order harmonic frequencies. The material nonlinearity can be quantified and correlated with material damage by determining the amplitude of higher order harmonics. Thus far, there are several applications of nonlinear ultrasonics to assess microstructural changes in metallic alloys, such as fatigue damage (49), (50), creep damage (51), (52), (53), radiation
damage (48), thermal aging (54), and cold work (56). The ultrasonic testing can be achieved by monitoring longitudinal waves (57), Rayleigh waves (58) or Lamb waves (49). Shui et al. (59) quantified the plastic damage in magnesium-aluminum alloy using longitudinal waves, and Pruell et al. (49) studied the plastic damage in aluminum using Lamb wave modes. Zeitvogel et al. (60) utilized nonlinear Rayleigh waves to detect stress corrosion cracking. Matlack et al. (48) reported a comprehensive review of the second harmonic generation method for detecting microstructural damage. In general, nonlinearity parameter $\beta$ increases with the increase of the density of microscopic heterogeneity, e.g., dislocation density or porosity. However, significant variations in the reported data and high errors in repeated measurements require more robust signal processing tool to decompose harmonic frequencies.

To extract the amplitudes of the fundamental and second harmonic frequencies, the most common signal processing method is to transform time domain signal into frequency domain by Fast Fourier Transform (FFT), and read the amplitudes of each frequency from the frequency spectrum. The major drawbacks of this approach are that temporal information is not preserved and that the transformation is ineffective in dealing with truncated signals or ones with discontinuity. If the frequency is constant in time, FFT can work properly (63). However, in the nonlinear ultrasonic testing, the objective is to find the complex nonstationary second order harmonic signals. Moreover, there are inherent characteristics of FFT that might affect the accuracy of signal decomposition. FFT uses some global basis functions and any perturbations in the transient signal in the time domain can dramatically affect the frequency spectrum (64); therefore, FFT is less accurate and unable to handle the local discontinuity in the time varying signal with transient properties (65). To solve this problem, short time Fourier transform (STFT) approach was implemented and introduced in the literature to overcome
the spatial limitations of FFT. In this method, an implicit assumption is made that the signal within the processing frame is repetitive and the signal can only be sampled for a limited time period (66). Time resolution is improved by decreasing the window size to calculate FFT; however, frequency resolution is reduced when FFT window has limited data points (67); thus, cannot provide good resolution in time and frequency simultaneously (68) (65) (69). As FFT cannot decompose non-stationary transient signal accurately, it is important to apply more robust signal decomposition approach to extract the acoustic nonlinearity parameter.

Goupillaud et al. (70) introduced the Wavelet Transform (WT) method to analyze the seismic signals simultaneously in time and frequency domain (70). WT offers an effective means in processing data (71) and has been applied to many signal and image processing applications. These investigations refer to different applications of WT, e.g. system identification and damage detection (72), damage localization (73), ultrasonic wave denoising (74), and mechanical fault diagnosis (75). In contrast to FFT, WT uses functions that are localized in both time domain and Fourier space called wavelets (76). By reconstructing signals into the mother wavelets, frequency components with the window of each wavelet can be identified. The window size in WT is a function of frequency. In higher frequency components, the window size gets smaller to maintain higher frequency resolution while in signals with lower frequency, higher frequency resolution is obtained by a larger window size (68). WT has been successfully applied in obtaining time-frequency images in both linear (77) and nonlinear (78) systems. It has been also developed in the form of Discrete Wavelet transform, Fast Wavelet Transform, and Continuous Wavelet Transform (79). Kim et al. (80) compared short time Fourier transformation and wavelet transformation and found out that the continuous wavelet transform is a promising method
to analyze the acoustic signals. Later in the thesis, we’ll conduct an error analysis to compare each method’s accuracy.

2.2 Simulations and predictions

The prediction of ultrasound wave in a heterogeneous medium is crucial due to many applications such as detecting damage in porous media, composites, granular material, or in diagnostic and therapeutic ultrasound (4). The heterogeneous components distort the wave resulting in changing the phase and generating higher-order-harmonics (HOH). Recently, there are more studies showing the relationship between heterogeneity and HOH.

Extensive studies have been done to experimentally determine the correlation between the acoustic nonlinearity parameter and the microstructural defects in the literature. These studies show that the morphological variations can influence microstructural damage nucleation to a significant extent (81) (82) (83) (84). Hikata et al. (85) showed that the dislocation in high-purity single crystal aluminum can contribute to both the second and third-harmonic generations. They discussed that tension-compression asymmetry and ultrasonic perturbation are necessary for the second-harmonic generation. However, the tension-compression asymmetry is not essential for generating the third-harmonics. In recent years, the study of HOH and their relation to microstructural heterogeneities have gained even more attention (39) (86) (87). Sablik et al. (88) studied the relationship between the microstructural attributes of steel and HOH in a magnetic induction test, and observed that monotonic decrease of third-harmonic amplitude occurs as the square root of dislocation density increases. They also observed a similar behavior for the first and the fifth harmonics. Shah et al. (89) considered concrete as a heterogeneous material and discovered the relation between the second and the third-harmonic ratios and damage severity in
concrete. They also reported that the third-harmonic is more sensitive to damage. Nonlinear ultrasonic guided waves have been employed by Liu et al. (90) for microstructural characterization of a steel hollow cylinder. They presented the effect of localized microstructural evolution on HOH. Chillara et al. (91) have addressed the issue of localized microstructure evolution in an inhomogeneous waveguide. They noticed that increase in the third-harmonic amplitude is proportional to the ratio of the plastic zone to propagation distance. In a later work, Chillara and Lissenden (92) also showed that tension-compression asymmetry led to even harmonic generation, while its symmetry resulted in odd harmonic generation.

Alongside experimental advancements, the numerical modeling has been employed to study the wave propagation in damaged materials. Shen and Giurgiutiu (22) studied Lamb wave propagation in a plate containing breathing crack using FEM. In their study, the crack was generated during cyclic fatigue loading of the plate. They introduced a baseline free damage index, which could be used to determine the density of cracks. Hong et al. (Hong et al. 2014) studied fatigue damage with the assumption of homogeneity of material and geometrical nonlinearities. They simplified the model by ignoring the non-uniform deformation and the localization of fatigue damage. Nonlinear Lamb wave simulation in thin plates was carried out by Wan et al. Wan2014. Their study only focused on single microcrack, and they proposed an amplitude ratio indicator for the detection of microcrack. Shen and Giurgiutiu (22) studied the generation of HOH due to the interaction of wave with a nonlinear breathing crack using two nonlinear FEM models: The element activation/deactivation method and contact analysis. They concluded that two methods could simulate the nonlinear behavior of breathing crack equally well. Despite close agreement between their results, no experimental data were reported to support their predictions.
They then developed an analytical predictive modeling to simulate guided wave interaction with damage which they concluded was faster than FEM. Considering the cumulative effect on the second-harmonic amplitude, Rauter et al. (93) modeled both geometrical and material nonlinearity. They concluded that the effect of cumulative second-harmonic is visible if the structure is excited at a suitable frequency extracted from the dispersion curve. Also, they noticed that the hyperelastic material modeling could appropriately model the micromechanically damaged material. Nonlinear ultrasonic response due to plastic deformation in welded joints was investigated by Xiang et al. (94). They considered the effects of dislocation length, geometrical, and plastic-induces nonlinearities within the acoustic nonlinearity coefficient. They observed that 4% plastic deformation results in an increase of 100% in the acoustic nonlinearity coefficient.

While much research has been placed in the second harmonic generation, the understanding and knowledge of HOH in detecting different damage types is still limited. Moreover, despite the studies in experimental assessment of second and third harmonics, few numerical analysis has been done to review and compare different harmonics. The fact that the solid continuum theory does not establish a well-grounded theory when dealing with mesoscale heterogeneity, such as the precipitants in metals is another motivation to predict the ultrasonic wave through numerical simulation.

2.3 **Finite element methods**

There are many studies investigating the relationship between damage and ultrasonic wave properties theoretically and experimentally. As described in previous chapter, acoustic nonlinearity parameter is the most popular tool for measuring the material nonlinearity which is proportional to the ratio of the second harmonic amplitude to the square of the first harmonic amplitude: $\frac{A_2}{A_1^2}$ (2) (3).
On the other hand, predictive modeling offers a means to gain insight into the relationship between the damage mode and the ultrasound signal. Shen and Giurgiutiu \cite{22} conducted FEM modeling of nonlinear Lamb wave in a plate with surface-breathing crack which are generated under cyclic fatigue loading. They studied the features of wave packets at receiver and introduced a baseline free damage index to assess the presence and severity of cracks. Hong et al. \cite{95} modeled fatigue damage with Abaqus/EXPLICIT™ software with the assumption that material and geometric nonlinearities are homogenous within the fatigued material, neglecting the fact that fatigue damage may be localized and non-uniformly distributed. Wan et al. \cite{96} modeled nonlinear Lamb waves in thin plates and proposed an amplitude ratio indicator for the detection of micro-cracks. However, they have only focused on single micro-crack type of damage. Shen and Giurgiutiu \cite{97} have used ANSYS software package to model the guided wave generated by interaction with a nonlinear breathing crack which have been modeled with two different techniques which compared quite well; however, no experimental analysis has been done to verify their predictions. Rauter et al. \cite{93} have modeled both material and geometrical nonlinearity with ANSYS considering the cumulative effect on second harmonic amplitude by choosing certain excitation frequencies and concluded that micro-mechanical damages can be modeled with appropriate nonlinear material model. Xiang et al. \cite{94} have studied nonlinear ultrasonic response due to plastic deformation in welded joints. They developed an FEM model and considered the effect of geometric and plasticity-induced nonlinearities and dislocation length on the acoustic nonlinearity parameter and observed 100% increase in the acoustic nonlinearity parameter under 4% plastic strain.
2.4 **Enriched numerical methods**

The development of the finite element method for wave propagation problems was the subject of a fair amount of research for so many years. Kohno et al. (98) presented a finite element scheme that merges advantages of the finite element and spectral methods. Low-order finite elements enriched with harmonic functions are used in this technique. The amount of enrichment is variable and can be represented by additional element degrees of freedom. One-dimensional time-harmonic multiscale wave problems with waves of dramatically different lengths in different regions and with wave conversions was solved. It was shown that, remarkably more accurate results can be obtained compared to using the traditional finite element for the solution of one-dimensional problems. For some decades, the general approach to enrich the conventional finite element basis functions with functions that can more accurately solve for the aimed solution, has been investigated (99). For the solution of specific problems this approach can be efficient. For instance, in the case of pipe analyses problem, specific functions were incorporated that are known to capture pipe ovalization effects more accurately (100). Utilizing these elements can lead to much more accurate and precise solutions both in linear and nonlinear analyses.

In the development of beam elements, the same technique has been adopted to include warping effects (101), or in the case of fluid flow analyses, the approach is used such that the flow conditions represented more accurately (102), whereas in solid mechanics, the method is applied to predict locally nonsmooth features such as voids and cracks (103). In all the methods mentioned, the nature of the solution pursued is incorporated in the solution space. Evidently, a suitable enrichment of the standard finite element functions is of concern whenever specific problems are dealt with.
Considerable research has been conducted on the development of numerical methods such as element-free methods to deal with high frequency harmonic wave propagation problems. Many researchers proposed the partition of unity finite element method (PUFEM) for solving high-frequency Helmholtz problems. Specific wave propagation solutions are incorporated in the solution space in this technique. In this method, the computational cost increases by adding the solution to the degrees of freedom of the interpolation function. To alleviate the ill-conditioning problem in PUFEM, the generalized finite element method (GFEM) was introduced which is an extension of PUFEM and was applied to time-harmonic acoustics. In this method, the homogenous solutions are multiplied by the standard FE shape functions.

Massimi et al. and Peterson et al. developed a discontinuous enriched method (DEM) in which nonconforming homogenous solution of governing problems are used for each element in addition to the FE approximations while continuity is enforced in the variational formulation. The enriched field is added to the polynomial rather than multiplied by it. The discontinuous approximation leads to diagonal mass matrix and saves computational cost. However, in these methods, the discontinuity between the elements need to be dealt with using methods such as penalty factors or Lagrange multipliers.

Other researchers proposed the spectral element method (SEM) as a generalization of FE in which higher order polynomials or harmonic functions are utilized in the solution space. In these methods, harmonic functions are used as basis functions and the problem is solved in the frequency domain. In this method, the accuracy is increased simply by enhancing the algebraic degree of these polynomials and adding to the degrees of freedom and thus increasing the computational cost.
Spectral Finite Element Method proposed later (26) proved to be very effective in solving high frequency wave propagation problems, however, due to the transformation of the governing wave equation to the frequency domain and solving the problem in frequency domain and transforming back to time domain spectral methods are computationally costly.

Ham et al. (112) has developed an enriched FE method which combines the advantages of standard FE and spectral FE by introducing additional degrees of freedom to the nodes. In this method, a ”priori” specific wave solution is not embedded and instead harmonic functions as a general solution of the wave is added to the standard FE interpolation functions. In this method, the mesh size must be fine enough or the number of harmonics used must be large enough to obtain accurate approximation.

Reproducing kernel particle method (RKPM) proposed by Liu et al. (113) uses a continuous reproducing kernel in a Lagrangian particle method to enhance both efficiency and accuracy of the other mesh-free methods. Liu et al. (114) applied RKPM in large deformation structural dynamics. Uras et al. (115) applied Reproducing Kernel Particle Method (RKPM) to acoustic problems. They used a multiple scale adaptive refinement technique through which they inserted additional particles in critical regions to enhance accuracy. The enrichment of finite element computations has been developed to enable the local treatment of computational domain with RKPM while solving the global problem with a standard finite element formulation(116).

Li et al. (117)(118) proposed a reproducing kernel hierarchical partition of unity method for efficient large scale computations. Classes of basis wavelet functions were introduced to form hierarchical partitions. These wavelet kernels were inserted into the primary interpolation function basis as multi-scale basis to numerically solve partial differential equations as refinements. They tested the so-called
pseudo-spectral basis by solving wave propagation and acoustic related problems. The method could efficiently capture the high frequency part of the solution where the regular FE method show deficiency and drastically improved the accuracy of the solution. However, the method requires careful tackling of ill-conditioning in the resultant mass and stiffness matrix.
CHAPTER 3

NONLINEAR ACOUSTICS

In this chapter nonlinear acoustic wave theory is reviewed and its application in nondestructive testing is discussed.

3.1 Theory and background

The governing equations for the motion of nonlinear wave propagation in elastic media can be derived from the conservation laws. With the stress-strain relationship for nonlinear material, the solution of the wave propagation can be obtained. Let $X$ be the original configuration of undeformed body $\Omega_0$ with density $\rho_0$ and $x$ the current configuration of deformed body $\Omega$ with density $\rho$. (Figure 1)

Figure 1. Original configuration $\Omega_0$ vs. current configuration $\Omega$
From the principle of the conservation of mass, we have:

$$\int_{\Omega_0} \rho_0 d\Omega_0 = \int_{\Omega} \rho d\Omega$$ \hspace{1cm} (3.1)

It can be shown that:

$$d\Omega = Jd\Omega_0$$ \hspace{1cm} (3.2)

where $J$ is the determinant of $F$, which is the deformation gradient. In the general form, $F$ is defined as below:

$$F = I + \nabla u$$ \hspace{1cm} (3.3)

where $I$ is the identity tensor and $\nabla u$ is the displacement gradient. Therefore [Equation 3.1] can be rewritten as:

$$\int_{\Omega_0} (\rho_0 - \rho J) d\Omega_0 = 0$$ \hspace{1cm} (3.4)

The linear momentum of a body in the current configuration is described as below:

$$P = \int_{\Omega} \rho v d\Omega$$ \hspace{1cm} (3.5)
In order to calculate the rate of linear momentum, the integral over current configuration needs to be converted to the original configuration:

\[
\frac{d}{dt} \int_{\Omega} \rho \mathbf{v} d\Omega = \frac{d}{dt} \int_{\Omega_0} \rho \mathbf{v} J d\Omega = \int_{\Omega_0} \frac{d\mathbf{v}}{dt} \rho_0 d\Omega = \int_{\Omega} \frac{d\mathbf{v}}{dt} \rho d\Omega \tag{3.6}
\]

Therefore,

\[
\frac{dP}{dt} = \int_{\Omega} \rho \frac{d\mathbf{v}}{dt} d\Omega \tag{3.7}
\]

In current configuration, the total force \( \mathbf{f}_t \) acting on the volume is:

\[
\mathbf{f}_t = \int_{\Omega} \rho \mathbf{b} d\Omega + \int_{\Gamma} \mathbf{t} d\Gamma \tag{3.8}
\]

where \( \mathbf{b} \) is the body force. The traction force on the surface \( \Gamma \) can be rewritten as:

\[
\int_{\Gamma} \mathbf{t} d\Gamma = \int_{\Gamma} \mathbf{n} \sigma d\Gamma = \int_{\Omega} \nabla \cdot \sigma d\Omega \tag{3.9}
\]

From the principal of balance of linear momentum, one can show:

\[
\frac{dP}{dt} = \mathbf{f}_t \tag{3.10}
\]
Substituting Equation 3.7, Equation 3.8 and Equation 3.9 in Equation 3.10 leads to:

$$\int_{\Omega} \rho \frac{d\mathbf{v}}{dt} d\Omega = \int_{\Omega} \nabla \cdot \sigma d\Omega + \int_{\Omega} \rho b d\Omega$$  \hspace{1cm} (3.11)$$

Equation 3.11 holds for all $x$ in $\Omega$. Therefore,

$$\frac{d^2 \mathbf{u}}{dt^2} = \nabla \cdot \sigma + \rho \mathbf{b}$$  \hspace{1cm} (3.12)$$

in which $\mathbf{u}$ is the particle displacement and $\sigma$ is the Cauchy stress tensor and can be obtained from the strain energy density function by:

$$\sigma = J^{-1} \mathbf{F} \frac{\partial W}{\partial \mathbf{E}} \mathbf{F}^T$$  \hspace{1cm} (3.13)$$

Under the finite deformation and the assumption of purely longitudinal motion, the deformation gradient takes the following form:

$$\mathbf{F} = \begin{bmatrix} l & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$  \hspace{1cm} (3.14)$$
in which \( l \) is the stretch in longitudinal direction. Considering the Green Lagrange strain tensor as below:

\[
E = \frac{1}{2} (F^T F - I)
\]  

(3.15)

The general strain energy density function for isotropic solids forms the following expression:

\[
W(E) = \frac{\lambda}{2} (trE)^2 + \mu trE^2 + A \frac{1}{3} trE^3 + B trE trE^2 + C \frac{1}{2} (trE)^3 + \ldots
\]  

(3.16)

where \( \lambda \) and \( \mu \) are Lamé parameters and \( A, B \) and \( C \) represent the third order elastic constants (TOE).

It can be shown in references that in the absence of viscosity, a single equation of motion for purely longitudinal motion can be written as:

\[
\frac{\partial^2 u}{\partial t^2} = c_l^2 \frac{\partial^2 u}{\partial x^2} g(\frac{\partial u}{\partial x})
\]  

(3.17)

where \( c_l \) is the linear wave speed and

\[
g(n) = 1 + (3 + \frac{c_{111}}{\rho_0 c_l^2})n + (3 + \frac{3c_{111} + c_{1111}}{\rho_0 c_l^2}) \frac{n^2}{2!} + \ldots
\]  

(3.18)
and when solved along its characteristics, it is found that the wave speed changes with the coefficient of nonlinearity as below:

\[ c = c_l + \beta \nu \]  

(3.19)

where \( \nu \) is the particle velocity and \( \beta \) has the following relationship with TOE:

\[ \beta = -\left(\frac{3}{2} + \frac{C_{111}}{2\rho_0 c_0^2}\right) \]  

(3.20)

where \( C_{111} = 2A + 6B + 2C \). A sinusoidal excitation \( u(0,t) = u_0 \sin \omega t \) produces the solution of Equation 3.17 as follows (Zarembo and Krasilnikov 1971):

\[ u = U_0 \sin \omega(t - \frac{x}{c_l}) + \frac{\beta}{4} k^2 U_0^2 x \cos 2\omega(t - \frac{x}{c_l}) + \frac{\beta^2}{8} k^4 U_0^3 x^2 \sin 3\omega(t - \frac{x}{c_l}) + \ldots \]  

(3.21)

The coefficients of second and third term in the equation above, indicate the second and third harmonic amplitude respectively. Therefore, the relative nonlinearity parameters attributed to the second and third harmonic ratio are defined as below:

\[ \beta' = \frac{A_2}{A_1^2} \]  

(3.22)

\[ \gamma' = \frac{A_3}{A_1^2} \]  

(3.23)
The Equation 3.22 and Equation 3.23 provides us a practical means to assess the damage state or characterize a material.
CHAPTER 4

SIGNAL PROCESSING TECHNIQUES

All this chapter has been previously published in (119). As described earlier in the previous chapters, nondestructive testing methods are more efficient and accurate using nonlinear ultrasound or nonlinear acoustic methods. The wave is distorted by presence of a damage and this distortion when quantified can be used as a measure to assess the material damage state. The accessibility for nonlinear acoustic methods is high. This allows fast investigation of complete objects, often done in one single test or more localized testing.

In earlier chapters, it is discussed that the most common measurement of the material nonlinearity is based on measuring the acoustic nonlinearity parameter $\beta$, which is proportional to the ratio of the second harmonic amplitude $A_2$ to the square of the first harmonic amplitude $A_1$ (2) (3). To date, there are several applications of nonlinear ultrasonics to assess microstructural changes in metallic alloys, such as fatigue damage (49) (50), creep damage (51) (52) (53), radiation damage (48), thermal aging (54) (55), and cold work (56). In order to measure higher harmonics’ amplitudes, the signal needs to decompose into different frequencies.

In this chapter, the Fast Fourier Transform (FFT) method and the proposed Wavelet Transform (WT)-based method are both implemented to decompose frequency amplitudes. The fundamental theories and equations of both signal processing methods are described and their advantages and disadvantages in extracting higher harmonics is reviewed. At the last section, the analytical solution of the
nonlinear longitudinal wave is used to verify the accuracy and effectiveness of WT in comparison to FFT.

4.1 Fast Fourier transform

FFT is the most commonly used signal processing tool to find the frequency content of transient signals based on the Fourier series expansion. The Fourier series of a time-dependent signal \( h(t) \) within the limit of \(-T < t < T\) is:

\[
h(t) = \sum_{n=-\infty}^{\infty} c_n e^{i\pi n T t}
\] (4.1)

\[
c_n = \frac{1}{2T} \int_{-T}^{T} x(t)e^{-i\pi n T t} dt
\] (4.2)

Where \( c_n \) corresponds to the nth coefficient in Fourier series. To process a signal with finite discrete values, Discrete Fourier Transform (DFT) is used. DFT of sequence \( h_n \) with \( N \) values is transformed to the frequency domain as:

\[
H_k = \sum_{n=0}^{N-1} x_n e^{\frac{-2\pi i nk}{N}}, k = 0, ..., N - 1
\] (4.3)

where \( k \) is the wave number and \( H_k \) is the corresponding sequence in the frequency domain. DFT is seldom utilized due to the large computational cost especially for large \( N \). Instead, by rearranging some multiplications and sums, a simple yet effective algorithm called Fast Fourier Transform (FFT) which is an efficient method to compute the Fourier transform, is used. FFT decreases the computational cost.
by reducing $N$, the number of points needed for computation from $2N^2$ to $2N\log_2 N$. If the frequency is constant in time, FFT works effectively (63). However, in the nonlinear ultrasonic testing, the objective is to find the complex nonstationary higher-order harmonic signals, which potentially poses a challenge for FFT.

A thorough review of FFT and its limitations are discussed in Section 2.1. In conclusion, FFT is ineffective to decompose non-stationary transient signal accurately, and it is important to apply a more robust signal decomposition approach to extract the acoustic nonlinearity parameter.

4.2 Wavelet transform

In contrast to FFT, WT uses functions that are localized in both real and Fourier spaces, called wavelets (76). By reconstructing signals into the mother wavelets, $\psi(t)$, frequency components with the window of each wavelet can be identified. Short time Fourier transform (STFT) requires a constant window length (called 'window size') , which slides through the time axis to calculate the FFT in each window and to add the temporal information of the signal into FFT (69). Unlike the STFT method, the window size in WT is not constant, and it is a function of frequency. In higher-frequency components, the window size becomes smaller to maintain higher frequency resolution while in signals with lower frequency, higher frequency resolution is obtained by a larger window size (68). A thorough review of WT and its characteristics are brought in Section 2.1.

The fundamental equation of wavelet transform can be expressed as:

$$w_n(s, \tau) = \int_{-\infty}^{\infty} h(t)\psi^*_{s,\tau} d(t)$$

(4.4)
Where $h(t)$ is the time domain signal and $(*)$ denotes the complex conjugate and $\Psi_{(s,\tau)}$ is called the daughter wavelet and can be characterized with the dilation and translation parameters, $s$ and $\tau$, respectively, as:

$$\psi_{s,\tau} = \frac{1}{\sqrt{s}} \psi\left(\frac{t-\tau}{s}\right)$$ (4.5)

The dilation and translation parameters $s$ and $\tau$, vary continuously to represent different times in the time domain signal and different contractions and dilations of the mother wavelet. The wavelet function should have zero mean and be localized in both time and frequency (120). In additional, the mother wavelets $\Psi(t)$ must satisfy the following admissibility condition:

$$\int_{-\infty}^{\infty} \left| \hat{\Psi}(\omega) \right|^2 d\omega < \infty \quad \hat{\Psi}(\omega) = \int \Psi(t)e^{-j\omega t}dt$$ (4.6)

where $\hat{\Psi}(\omega)$ is the Fourier transform of $\Psi(t)$. Among many wavelets, Morlet wavelet has been shown to have the best temporal and spatial resolution (75). In this study, the complex Morlet wavelet obtained by the product of a complex exponential and a Gaussian function is selected as the mother wavelet. The exponential decay in complex Morlet results in very precise time localization. This wavelet provides the best resolution in time and frequency; therefore, it is the most suitable wavelet for spectrogram analysis (121)(122). The complex Morlet wavelet has the following forms in the time and frequency domains (123):
\[ \Psi_M(t) = \frac{1}{\sqrt{\pi \omega_b}} e^{2i\pi \omega_c t} e^{-\frac{t^2}{\omega_b}} \]  

\[ \Psi_M(\omega) = e^{\pi^2 \omega_b (\omega - \omega_c)^2} \]  

where \( \omega_b \) and \( \omega_c \) are the parameters controlling the frequency bandwidth and the central frequency, respectively. Figure 2 shows the complex Morlet wavelet with the central frequency of 1.5 Hz and bandwidth of 1 Hz.

![Figure 2. Complex Morlet with central frequency of 1.5 Hz and bandwidth of 1 Hz, (a) time domain (b) frequency domain.](image-url)
4.3 Acoustic nonlinearity parameter obtained by WT-based method and FFT-based method

In this section, the acoustic nonlinearity parameter obtained by both FFT and WT is compared for a one-dimensional nonlinear wave problem, according to the analytical solution shown in Equation 3.21. The time-frequency spectrogram is first obtained with the selected mother wavelet, after the time-history signal is recorded, and then wavelet coefficients (amplitude) of the first and second harmonics with respect to time, $A_1(t_i)$ and $A_2(t_i)$, respectively, are extracted. Here the subscript $i$ denotes the $i$th data point. In this study, the time history signals consist of 2048 discrete points. The first harmonic frequency occurs at 2.25 MHz, and the second harmonic frequency is twice the first harmonic at 5 MHz, as shown in Figure 3. Two red lines in Figure 3(c) show the positions of first and second harmonics on the wavelet spectrum. Once the two modes are decomposed, the acoustic nonlinearity parameter can be obtained by $\beta(t_i) = \frac{A_2(t_i)}{A_1(t_i)}$. This algorithm provides a detailed variation of $\beta$ values and how it varies with time due to different incidents with respect to time.

The acoustic nonlinearity parameter $\beta$ is an inherent material property and should not be dependent on the excitation amplitude or frequency. However, if in the signal processing the errors from the extraction of $A_1$ and $A_2$ are of the same order, the error of calculated $\beta$ depends on the $A_2$ value. This can be concluded from the sensitivity analysis of $\beta$ formulation, which demonstrates the error $\frac{A_2 \pm \epsilon}{(A_1 \pm \epsilon)}$ from Equation 3.22 is in the order of $O(2 \frac{\epsilon}{A_1} + \frac{\epsilon}{A_2})$, where $\epsilon$ is the error from signal processing of $A_1$ and $A_2$. The error of the calculated $\beta$ is amplified when $A_2$ is much smaller than $A_1$, which is typically the case as the amplitude of the second harmonic frequency due to the microstructural damage is weak. Therefore, it is imperative that the amplitudes of $A_1$ and $A_2$ for nonlinear UT techniques be accurately measured and extracted.
To verify the effectiveness of the wavelet-based schemes for calculating the acoustic nonlinearity parameter, the analytical solution in Equation 3.21 is employed as the input signal to completely remove measurement errors. The values of material parameters used are as follows:

The input signal $u(x, t)$ is generated according to Equation 3.22 with various input amplitudes, $u_0$, and a fundamental frequency of 2 MHz. Figure 3 a, b and c show $u(x, t)$ for a given $u_0$, its time-frequency spectrogram from WT, and its frequency domain from FFT, respectively. The variables to perform WT are 100 MHz sampling rate and the scale of 1000, whereas the parameters to calculate FFT are 100 MHz sampling rate, and 16384 data points. In this study, the complex Morlet with 1.5 Hz central frequency $\omega_c$ and a bandwidth $\omega_b$ of 1 Hz is implemented. The scale $a$ in Equation 4.9 is
TABLE I

<table>
<thead>
<tr>
<th>Material parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$ (Pa)</td>
</tr>
<tr>
<td>$3.51 \times 10^{11}$</td>
</tr>
</tbody>
</table>

increased from 500 to 10k and the convergence in the spectrogram is reached at the scale of 5000 or greater. The pseudo frequency $F_a$ is 30 kHz with a scale of 5000 and sampling frequency of 100 MHz (124).

$$F_a = \frac{\omega_c}{a\delta}$$ (4.9)
Figure 4. A comparison of nonlinearity parameter calculated by WT vs FFT
CHAPTER 5

HIGHER HARMONICS AND THEIR RELATIONSHIP TO MICROSTRUCTURAL FEATURES

All this chapter is submitted to be published in Ultrasonics journal. In this chapter the numerical studies conducted in order to find the relationship between microstructural variation and higher harmonic emergence have been discussed.

5.1 Introduction

In Chapter 2, we discussed the necessity of predicting ultrasound waveform in heterogenous materials. In particular, the use of nonlinear ultrasound in assessing microstructural evolution enables the prediction of the remaining life of the structure earlier. There are many cases showing the initiation of a macroscale damage by microscale evolution such as the process of incipient fatigue damage in metals (125) (126). The detection and characterization of variety of microstructures such as dislocation density, precipitates and embrittlement can provides us with information regarding the structure’s safety and shifting the earliest possible remaining life prediction (91). Lately, high amplitudes of third harmonics are reported in the presence of different damages such as cracks and grain boundaries (89). The current study is aimed to address the issue of damage detection by nonlinear ultrasonics in heterogeneous media numerically. In this work, the second phase heterogeneities are explicitly modeled to study the correlation of mesoscale and micro scale heterogeneity and higher order harmonics. Accordingly, a heterogeneous material is constructed, with the Aluminum 1100 to represent the homogeneous part and
inclusions which differ in material property, size and volume fraction and study the influence of plastic
deformation on the nonlinear acoustic parameters. To this end, several different Representative Volume
Elements (RVEs) are fashioned to create blocks representing the neck area of a dog bone sample. RVEs
are chosen such that the macroscopic constitutive model can represent the average constitutive response.
Therefore, they are large enough so that their variations are statistically insignificant yet smaller than
the wave length of ultrasound.

To obtain the nonlinear acoustic parameter, the time domain response obtained from the numerical
model needs to be transformed into to frequency domain. In order to enhance accuracy, Wavelet Trans-
form is used to calculate the frequency domain response. We also study the mesh sensitivity of finite
element analysis in the nonlinear wave propagation and suggest a minimum element size per wavelength
to control the error of the calculated nonlinear acoustic parameter and validate our model with the ana-
lytical solution of nonlinear wave. The results are validated by several experimental studies done in the
past.

5.2 Methodology

In previous chapters, it was described how harmonic amplitudes are related to the nonlinearity of
materials. Moreover, the microstructural complexity can govern the mesoscale properties such as ductil-
ity, nonlinearity, fracture toughness and overall mechanical behavior. In this section, the development of
a numerical simulation capable of assessing the relationship between higher harmonics and heterogene-
ity in material is described. In this framework, it is assumed that the mesoscale model is constructed
from a simplified form of micrographs.
There exist numerous techniques to produce digital data from microstructure. Scanning electron microscopy (SEM) and Optical microscopy are among these methods. The geometry and properties of the microstructure are extracted from the digital data by different image segmentation techniques. The segmentation approach can enable us to conduct numerical analysis on the digital image of the microstructure. In the process of digitalized data incorporation into the numerical model, it is important to ensure the numerical microstructure is statistically identical to the actual microstructure. In order to make this happen and have a realistic macroscopic modeling considering microscopic evolution, the model is represented as an assemblage of independent elements, interacting with one another. The assumption is that the material can be approximated as assemblies of discrete elements attached together by different properties.

Through this scheme, heterogeneities are modeled in such a way that almost any heterogeneous model can fit. Industrially relevant cases from the precipitates in Aluminum’s second phase to the aggregates in concrete can be simulated through varying the heterogeneity size, material properties and volume fraction. In this way, the size of each element can equate with the size of second phase precipitates or with larger heterogeneities through blocks of elements. The heterogeneous blocks then are randomly distributed over the whole domain. The predictive capability of the computational model using simplified representation of microstructures is then used to simulate wave propagation, thus measuring the nonlinearity parameter $\beta'$.

Predicting the mechanical response of such materials from the information of their microstructure and behavior of single components has been a challenging issue. Therefore, homogenization methods will be discussed in future works.
Modeling the material is one of the main challenges in constructing an accurate numerical simulation and better predicting the nonlinearity parameter. For this purpose and as the base simulation, Aluminum 1100 has been considered to have a heterogeneous microstructure. This heterogeneity in the microstructure is portrayed by fine spherical precipitates, intermetallics and the presence of micro-scale second phase particles in the matrix. Scanning the Aluminum sample will give us the chance to access the statistical data regarding the second phase particles using ImageJ™.

Figure 5. Left: Al1100 Optical Micrographs (200X), Right: Numerical microscale model

According to these statistics we can see that there is a volume fraction of 2% for second phase particles. In another study ([127], it has been shown that concrete can have a volume fraction up to 60% aggregate to texture. In this research, several models have been prepared and tested using different heterogeneity parameters including values mentioned above.
In order to introduce the plastic deformation, a loading and unloading stage is conducted. The unloading response in heterogeneous materials is much more complex than the conventional recovery process observed in single-phase metals. The reason is that the plastic deformation is observed to occur during the unloading process \cite{128}. In order to capture the mechanical behavior in the microscale, an isotropic plasticity material model is used. In this method, the plasticity calculations are based on the classical metal plasticity model with isotropic hardening. For this matter, experimental test data for Aluminum 1100 are used along with the von Mises yield criterion, which can be expressed as follows:

\[ J_2 = \frac{1}{2} \text{tr}(S \cdot S) \]  

(5.1)

where \( S \) is the deviatoric part of the stress tensor:
\[ S = \sigma - \frac{1}{3} (\text{tr}(\sigma)) I \] (5.2)

Hence, the yield function is described as:

\[ f(J_2) = \sqrt{J_2} - \alpha(\epsilon_p) \] (5.3)

where \( \alpha \) is the material’s yield stress under pure shear which in turn is a function of the plastic strain \( \epsilon_p \). It is assumed that this material model has the capability to capture dislocations happening during plastic deformation.

Using this method, one can determine the property of the material using heterogeneity once and only at the beginning the analysis using micrographs. By doing so, one can forward predict the \( \beta' \) change due to plastic deformation. Taking advantage from this forward prediction, there is no need to observe microstructurtral evolution and dislocation density variation or rearrangements during the plastic deformation process.

5.3 Validation and convergence study

Generally, a finer mesh will lead to better results; however, it will have a negative effect on efficiency. For nonlinear analysis, it is essential to consider a maximum limit for the element size to ensure accuracy. It has been suggested to have at least 20 elements per wavelength to avoid numerical dispersion and dissipation error (22):
element size: $\Delta h \leq \frac{\lambda}{20}$  \hspace{1cm} (\lambda = \text{wavelength}) \hspace{1cm} (5.4)

time step size: $\Delta t \leq \frac{1}{20f}$  \hspace{1cm} (f = \text{frequency}) \hspace{1cm} (5.5)

In order to make sure the mesh size and time step size used is satisfactory, a convergence study is done. A homogeneous three dimensional model is constructed and its boundary conditions are enforced such that the model imitates a one dimensional problem (see Figure 7). For a 2MHz signal, according to Equation 5.4, the calculated maximum element size and time step are 0.3 mm and 0.05 $\mu$s. Therefore, a mesh size of 0.08 mm and a time step of 0.001 $\mu$s are sufficient to ensure accuracy and capture higher harmonics.

In order to define the Landau and Lifshitz’s hyperelastic material model (129), a User Material (UMAT) script is written and incorporated into the implicit finite element code Abaqus™. Within the UMAT, the system of nonlinear equation is solved by the Newton-Raphson method given the incremental strains. Proper definition of stress and the Jacobian is required. Knowing strain energy density, with the following relationship the Second Piola-Kirchhoff stress tensor can be defined:

$$S = \frac{\partial w}{\partial E}$$  \hspace{1cm} (5.7)
Following Equation 5.7 and Equation 3.16, the second Piola-Kirchhoff stress tensor can be expressed as below:

$$
S = \lambda tr\mathbf{E} + 2\mu \mathbf{E} + C tr\mathbf{E}^2 + B tr\mathbf{E}^2 + 2B(tr\mathbf{E})\mathbf{E} + A tr(\mathbf{E}^2)
$$

The material properties used for Aluminum is as below:

A sine wave is applied uniformly at one edge and the results are measured at the nodes on the edge across from it and then averaged. Comparing with the analytical solution, it can be demonstrated in Figure 8 and Figure 9 that the mesh used is sufficient to preserve accuracy of the nonlinear wave:
TABLE II

Hyperelastic material property [Aluminum]

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( A(Pa) )</td>
<td>( 3.51 \times 10^{11} )</td>
</tr>
<tr>
<td>( B(Pa) )</td>
<td>( 1.444 \times 10^{11} )</td>
</tr>
<tr>
<td>( C(Pa) )</td>
<td>( 1.028 \times 10^{11} )</td>
</tr>
<tr>
<td>( \rho(\frac{kg}{m^3}) )</td>
<td>( 2700 )</td>
</tr>
<tr>
<td>( \lambda(Pa) )</td>
<td>( 51.05 \times 10^9 )</td>
</tr>
<tr>
<td>( \mu(Pa) )</td>
<td>( 26.32 \times 10^9 )</td>
</tr>
</tbody>
</table>

Figure 8. Numerical Vs. Analytical solution of nonlinear wave

An additional convergence study is performed to evaluate the mesh size accuracy in the presence of heterogeneity. In this study, two 2-dimensional heterogeneous models have been simulated, having the exact same material, geometry, loading and heterogeneity characteristics. One of them is spatially discretized with the element size used mentioned in the previous section, while the second model is discretized with elements half of the size utilized before. Again, as can be observed in the results shown in Figure 10 and Figure 11, the utilized element size of 0.08 mm meets the requirements of the accuracy of the solution:
5.4 Numerical damage detection in statistically variable heterogeneous media under plastic deformation

FEM commercial software Abaqus™ is used to model the nonlinear wave propagation through the specimen. To model a three dimensional dog bone specimen, the size of the model has been reduced to the neck part, and symmetric boundary conditions are used to decrease the computational cost of the numerical simulation. The model is discretized by first order reduced integration linear hexahedral elements (C3D8R). In order to introduce different stages of damage in the material, plastic deformation is applied at 1%, 2%, 3% and 4% strains. The applied strains are deactivated for a sufficient amount of time in order to simulate the unloading stage and then the wave propagation stage is modeled.
The excitation of a 10 cycle tone burst Hanning window with the frequency of 1MHz is realized through a circular area to replicate the transducer. The expression of the excitation is shown in Figure 12:

\[
f(t) = \sin(2\pi ft)(0.5(1 - \cos(2\pi f \frac{t}{N})))
\]

The temporal and spectral waveform is plotted: Implicit time integration dynamic simulations were performed and the resulting waves were output and averaged exactly at the opposite side of the transducer. Figure 13 shows the geometry with associated mesh of the used model:

The heterogeneities are considered as 27 groups of different material models. Each of these material heterogeneity models has been considered to have 5 different random positions through out the model. In this study, different aspects of heterogeneities including volume fraction, standard deviation and heterogeneity size are considered as variables. The aim of this study is to observe the correlation between
each of these factors and the production of the higher harmonic. Moreover, the importance factor of each of these variants is discussed. The following table represents the guide for this parametric study:

The heterogeneities are considered as 27 groups of different material models. Each of these material heterogeneity models has been considered to have 5 different random positions throughout the model.

In this study, different aspects of heterogeneities including volume fraction, standard deviation and heterogeneity size are considered as variants. The aim of this study is to observe the correlation between each of these factors and the production of higher harmonic. Moreover, the importance factor of each of these variants is discussed. The following table represents the guide for this parametric study:
According to [119] Wavelet Transform (WT) is a more accurate tool to convert the signal to the frequency domain and measure nonlinearity. Therefore, the results are post-processed by WT, considering the complex Morlet wavelet as the mother wavelet $\Psi(t)$:

$$
\psi_M(t) = \frac{1}{\sqrt{\pi \omega_b}} e^{i2\pi\omega_b t} e^{-\frac{t^2}{\omega_b}}
$$

(5.10)
TABLE III

<table>
<thead>
<tr>
<th>Heterogeneity Size</th>
<th>Volume Fraction</th>
<th>Standard Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 element</td>
<td>2%</td>
<td>10%</td>
</tr>
<tr>
<td>4 elements</td>
<td>10%</td>
<td>30%</td>
</tr>
<tr>
<td>18 elements</td>
<td>20%</td>
<td>60%</td>
</tr>
</tbody>
</table>

\[ \psi_M(\omega) = e^{\pi^2 \omega_b (\omega - \omega_c)^2} \] (5.11)

where \( \omega_b \) and \( \omega_c \) are the parameters controlling the frequency bandwidth and the central frequency, respectively. The received time-domain signals from a pristine plate and damaged plates with plastic strains up to 4% are illustrated in Figure 14. The series of figures are pertinent to one of the 27 simulations.

As observed in these figures, the third harmonic mode’s amplitudes are greater than those of the second harmonic and have more explicit waveforms. From the above figures the second and third harmonic nonlinearity factors are derived for each time instance according to Equation 3.22 and Equation 3.23 and plotted as below:

It is worth mentioning that the comprehensive description of measuring nonlinearity using the aforementioned method can be found at (119). As can be observed in Figure 15, an average quantity is considered to represent the magnitude of second and third order nonlinearity parameters in a certain time period. These calculations are repeated according to the statistical study guide for different heterogeneity.
Figure 14. Time-domain signals of pristine to 4% plastic strains

ity parameters and at different stages of damage and the second and third harmonic nonlinearities are plotted and shown in Figure 16 and Figure 17.

The plots in Figure 16 and Figure 17 are quite informative. It is clear that the result of second-harmonic based nonlinearity cannot provide the link to the plastic strain and $\beta'$ in the material. There is no obvious pattern, especially when dealing with lower amounts of volume fraction and heterogeneity sizes. In all these cases, no matter how much the standard deviation rises, there is no significance change in $\beta'$. However, moving towards higher amounts of volume fractions and heterogeneity sizes, the standard deviation also makes considerable difference, and in the last model, an increase of up to 50% is observable.

On the other hand, the third harmonic nonlinearity parameter is much more sensitive to any heterogeneity parameter than the second harmonic nonlinearity. Even in the first model with volume fraction
of 2% and very fine heterogeneity, higher standard deviation clearly shows higher nonlinearities. In fact, even with different positions of heterogeneities, there exists a distinct bundle for each corresponding standard deviation. Moving towards higher volume fractions and heterogeneity sizes, the increase of $\gamma'$ is distinctly noticeable and in the last model, an increase of up to 200% is seen. Therefore, in the case of the third harmonic-based measurement of nonlinearity, all the heterogeneity characteristics play an important role. In particular, standard deviation is the most effective factor, especially when dealing with smaller amounts of volume fraction and finer heterogeneities. Even for the cases that nonlinearity is measured by second harmonic ratio, it can be observed that samples with higher standard deviations show an increasing trend and have greater magnitudes, whereas varying the heterogeneity size or volume fraction cannot affect the second harmonic ratio. This can further demonstrate the presence of voids in cases where there is creep or granular material can affect the third harmonic ratio the most regardless
of their size or volume fraction. Thus, third harmonic detection can be a more effective tool to predict damage.

5.5 Validation

Experimental studies to demonstrate the relationship between damage in structures and higher harmonics have been conducted for a few decades. In this study the relationship between microstructural variations in a heterogenous medium and second and third harmonics are of particular interest. The results in the previous section depicted an enhanced capability of the third harmonic nonlinearity calculation to detect the flaws in heterogenous media. However, only recently the significance of third harmonics in diagnosis of microstructural evolution has only recently been explored. One of the earliest studies regarding the aforementioned relationship was done by Hikata at 1966 (85). In this study the generation of ultrasonic second and third harmonics due to dislocations are discussed. The authors have measured the amplitude of third harmonics as well as second harmonics as a function of impurity content, static bias stress, plastic deformation and amplitude of the fundamental wave. They concluded that the third harmonic lends itself to study of the interactions between dislocations and point defects more directly than the second harmonic. Moreover, it was shown that amplitude of third harmonic is dependent on dislocation loop length and small amount of plastic deformation leads to a considerable increase in the effective dislocation loop, hence increasing the third harmonic mode’s amplitude.

In a later study (130) Elbaum and Hikata have investigated two anharmonic properties of vibrating dislocations: lattice and dislocation. They analytically showed that in a solid containing dislocation, the dislocation component is much larger than the lattice component for the third harmonic. They
therefore concluded that by investigating the third harmonic, it is possible to obtain detailed information on dislocation dynamics.

Another experimental study on plain concrete (131) demonstrated that the third harmonic in the case of microcracks is an indicator of damage level, especially in the models with quadratic nonlinearity. In another study on composite materials (132), Meo showed the dependence of both second and third harmonics on damage level, however, the third harmonic shows more sensitivity.

Later on Shah et al. (89) calculated the second and third harmonic at different damage and power levels on concrete. They noted that abnormally high levels of the third harmonic are observed in the presence of cracks and grain boundaries. Considering their experimental studies, the third harmonic has greater level of amplitudes for different levels of water to cement ratio in concrete. In this case, both second and third harmonics showed extraordinary sensitivity. This fact is in line with the present study since concrete could have up to 60% standard deviation and 20% volume fraction with large heterogeneities, and hence easily comparable to the diagrams shown in Figure 16 and Figure 17. From the numerical study conducted in previous section, it is clearly observed that in the case of severe heterogeneity characteristics, both the second harmonic and third harmonic demonstrate considerable sensitivity, with the third harmonic showing a stronger correlation.

One of the most relevant studies to the numerical study conducted in this work is the experimental study of Lissenden et al. (133) on Aluminum plates. They have shown that the plastic deformation increases the third harmonic amplitude by up to a factor of five. In their study, the authors reported the results of another study on an Aluminum 1100 plate that was plastically deformed up to 1.7% without registering any significant change in the plastic strain level.
Moreover, in a later study by Chillara et al. [92] it is demonstrated that for an elastoplastic spring mass system, the time-domain signal is symmetric and the frequency domain contains all the odd harmonics but not any even harmonics. They discuss the fact that the tension-compression asymmetry is responsible for even harmonic generation. Ideally, the numerical model used in the current study follows an elastoplastic material model relationship, hence there is no bias in tension and compression of the model, preventing the generation of second harmonics due to material nonlinearity.

Third harmonics have been studied more recently with a variety of wave types. Liu et al. [90] studied the shear horizontal and Rayleigh lamb waves in a mathematical approach with the objective of predicting the cumulative behavior of the third harmonic due to interaction of two collimated waves in an isotropic elastic plate with cubic nonlinearity. They provide theoretical guidance for primary mode selection in order to cumulatively generate third harmonics due to material microstructure change. They showed that all points on the primary dispersion curves are internally resonant with third harmonics, which is not the case for second harmonics. While it is worth mentioning that in a numerical study [91] conducted later on the influence of microstructure evolution on second harmonics in guided waves, it was noticed that even though all the conditions for a cumulative second harmonics were met, the second harmonic did not accumulate linearly with propagation distance, and the researchers have related this phenomenon to the inhomogeneous nature of the plate.

All in all, the authors believe the above analytical and experimental studies can be valuable points of reference to validate the current numerical study.
5.6 Conclusions

In this paper, the correlation between higher harmonics and different heterogeneity characteristics and randomness has been established using several numerical models. Different heterogeneous models were constructed and simulated in Abaqus™. The heterogeneity in material has been modeled explicitly as blocks of elements and an elastoplastic material model is taken to represent the dislocation in the model. Heterogeneity characteristics including the volume fraction, the standard deviation, heterogeneity sizes and their positions throughout the media are set to different values and the nonlinear ultrasonic testing conditions are modeled to see the effect of different heterogeneous characteristics on the higher harmonics. The spatial discretization of the models is verified with the analytical solution of the nonlinear wave propagation in a hyperelastic medium in which the material model is written in a UMAT script and incorporated in the simulation. Two-dimensional heterogeneous models are also used for another convergence study. Harmonic generations are then investigated. The second harmonic nonlinearity parameter $\beta'$ and the third harmonic nonlinearity parameter $\gamma'$ are calculated. It is evident that in the case of heterogeneity, the third harmonic is more sensitive than the second harmonic. There is a distinct upward trend observed in $\gamma'$ calculations with respect to increasing plastic strain, whereas, $\beta'$ does not show sensitivity with increasing plastic strain. These results are in line with previous experimental studies in the literature. In addition, samples with higher standard deviation in their material property show a higher $\beta'$ overall. Also, the contribution of standard deviation to the harmonic generation is higher than the volume fraction and heterogeneity size. Nonetheless, the effect of volume fraction and heterogeneity size is not negligible. All in all, there is a direct relationship between increasing all heterogeneity attributes and the third harmonic. This is essential in detecting damage due to
plastic deformation in heterogeneous material. It was found that the third harmonic generation is a much
greater asset when dealing with heterogeneous media. Moreover, using elastoplastic material modeling
along with explicit modeling of heterogeneities provides the analyst with the opportunity of utilizing the
same microstructure under different types of loading and monitoring the change of microstructure. It
is worth mentioning that the nonlinearity of the material is solely due to heterogeneities and there is no
other source of nonlinearity. Multiscale numerical modeling of heterogeneous media using micrographs
and improving the numerical model to capture higher harmonics efficiently are the next steps for this
research.
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<th>vf=20%</th>
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<tr>
<td><img src="image9" alt="Graph 9" /></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Figure 16. 2nd harmonic based nonlinearity ($\beta'$) vs. Plastic strain
Figure 17. 3rd harmonic based nonlinearity ($\gamma'$) vs. Plastic strain
CHAPTER 6

INFLUENCE OF MESOSCALE AND MACROSCALE HETEROGENEITIES IN METALS ON HIGHER ORDER HARMONICS

This chapter is submitted to be published in the "Journal of Nondestructive Evaluation".

Nonlinear ultrasonic techniques are known to be sensitive to material nonlinearity, some of which can be attributed to microstructural damages. The material nonlinearity is observable in the ultrasonic signal through the generation of higher-order-harmonics (HOH). The HOH generation, however, can be triggered by many sources. Any variation in the micro-, meso-, and macroscopic scales of the structure may collectively lead to HOH generation.

This chapter presents a finite element approach with mesoscale heterogeneities explicitly modeled for the nonlinear wave propagation. The aim of this study is to understand HOH generation due to the non-mesoscale variation and non-uniform deformations introduced by the uniaxial tensile test. The study is divided into two parts: First, the effect of non-uniform plastic deformation resulted by geometrical variation of structures on HOH is studied. Next, the effect of non-uniformity due to mesoscale variations on HOH is analyzed. For this purpose, wavelet-based algorithms are applied to measure the acoustic nonlinearity parameter. The numerical studies and predictions are crossly validated with nonlinear ultrasonic experiments and microscale imaging, including X-ray Diffraction (XRD) scanning. Numerical and experimental studies both indicate that non-uniform variations in different length scales affect the generation of both the second and the third-harmonics, and that both second- and third-harmonics acoustic nonlinearity parameters grow with the increase of plastic strain level. How-
ever, the third-harmonics acoustic nonlinearity coefficient is more sensitive when micro-, meso- and macrostructural variations exist. Accordingly, this parameter is a more beneficial indicator of nonlinearity in materials when non-uniform deformation is present.

6.1 Introduction

Nonlinear ultrasonics testing (NLUT) has been applied to the detection of microstructural changes in the earliest stage of degradation in metallic structures due to fatigue and creep \(^{(53)}\). One of the successful methods is based on the correlation between the higher-order-harmonics (HOH) generation and materials nonlinearity \(^{(134)}\). HOH generation, however, can be attributed to many different sources, including, dislocation, grain boundary, precipitates, microcracks, voids/defeats, surface roughness/boundary or geometry of the specimen. The sources can be generally viewed as variations at three different length scales, namely, a scale much smaller than the wavelength (referred to as microscale), one comparable with the wavelength (mesoscale), and one much larger than the wavelength (structural level). In practice, all the sources contribute to the HOH generation, and thus the experimental identification of the main source of HOH generation is challenging. While there are many experimental studies into NLUT in the literature, few investigations have used numerical techniques to predict the relationship between material nonlinearities and HOH. Numerical modeling offers a means to gain valuable insight into the relationship between different damage modes such as non-uniform deformation and the ultrasound signal. The numerical model for NLUT is based on finite amplitude wave equation, and the correlation between HOH and nonlinear material properties is established using continuum theory with nonlinear elastic constitutive models. Therefore, the continuum-based nonlinear constitutive model is suited to describe the mechanical behavior of materials with microscale heterogeneities. However,
when mesoscale heterogeneities exist and contribute to a non-negligible volume fraction in material, their effect on wave propagation cannot be fully captured by the continuum-based constitutive models. Moreover, the structural-level geometry and loading condition induce non-uniform plastic deformations, which in turn introduce non-uniform microscale damages, and further complicate the tasks to understand the sources of HOH generation. This study presents a finite element approach with mesoscale heterogeneities explicitly modeled for the nonlinear wave propagation. Crossly validating with nonlinear ultrasonic experiments and microscale imaging, the aim of this study is to understand HOH generation due to the non-mesoscale variation and non-uniform deformations introduced by the uniaxial tensile test.

In the literature, non-uniform stress distribution at the structural level can occur near the intersection of different geometric forms, whereas the precipitations along grain boundaries can be attributed as the dominant source of the non-uniform deformation and thus material nonlinearity at the microstructural level \( (135) \). As the level of deformation increases, dislocations begin to appear, which leads to release of the stored energy and also redistribution of internal stress field. Accordingly, plastic deformations and damage growth occur near the material inhomogeneity or morphological variation. When exceeding a certain threshold, damage emerges as the form of microcracks, which ultimately nucleate and form macroscopic cracks in the material. Microstructural defects or heterogeneities lead to further nonlinearity in material and scatter and distort the ultrasonic wave \( (39) (40) (41) \). There are different approaches to measure the nonlinearity using ultrasonic method. As the fundamental wave mode propagates in the material, the interaction of this wave with microstructural damage generates HOH frequencies. Thus, the material nonlinearity can be quantified and correlated with material damage by determining the amplitudes of HOH. Acoustic nonlinearity parameter is one of the popularly used tools for measuring the
material nonlinearity which is proportional to the ratio of the HOH amplitude to the square or cube of the first harmonic amplitude. A thorough literature review of the numerical and experimental studies to determine the correlation between the acoustic nonlinearity parameter and the microstructural defects and wave propagation in damaged material is given in Section 2.2.

Despite numerous studies on the second-harmonic generation, the contribution of different damage types on the HOH generation is still unknown. This present study experimentally and numerically examines the effects of nonlinearity caused by non-uniform deformation, which are emerged either by geometrical variations at the structural level and/or variations at the microstructure of material due to plastic deformation to the generation of HOH in aluminum. The sensitivities of the second- and third-order harmonics to geometric and materials nonlinearities are compared.

6.2 Numerical modeling

The governing equations of the physical problems considered, the finite element procedure, and the important attributes of the numerical solution technique have been brought in Chapter 3 and Section 5.2.

6.3 Experimental design

6.3.1 Materials preparation

Aluminum 1100 with the composition in Table IV was selected to investigate the effects of non-uniform deformation and plastic deformation on HOH. Nine samples were machined from a 6.3mm thick cold rolled plate according to ASTM standard E8 to the dimensions shown in Figure 18. All samples were stress relieved at 250°C for 15 min prior to tensile testing. An MTS tensile machine, model 1125 was used for the tensile tests using a strain rate of 2.54 mm/min. The first sample was tested to failure to obtain the stress-strain curve and to determine the yield and tensile strengths, as well as
the Young’s Modulus and the strain at the ultimate tensile stress (UTS), which are reported in Table 2.

The remaining samples were plastically deformed between 0.5\% and 4\% at 0.5\% strain increments to produce different uniform plastic deformations through the gage area to avoid non-uniform plastic deformation at the onset of necking at the ultimate tensile strength (UTS). Figure 19 shows the stress-strain curves for all the samples tested. Figure 20 shows the two sections from gage length and the shoulder area, which were used in both numerical and experimental studies to understand the influence of uniform and non-uniform deformation on acoustic nonlinearity coefficients, respectively.

**TABLE IV**

Typical chemical composition of Aluminum 1100

<table>
<thead>
<tr>
<th>Aluminum 1100</th>
<th>Al</th>
<th>Cu</th>
<th>Mn</th>
<th>P</th>
<th>Si+Fe</th>
<th>Zn</th>
<th>Others</th>
</tr>
</thead>
<tbody>
<tr>
<td>Weight%</td>
<td>99 (min)</td>
<td>0.05 – 0.2</td>
<td>0.05 max</td>
<td>0 – 0.03</td>
<td>0.95 max</td>
<td>0.1 max</td>
<td>0.15 total</td>
</tr>
</tbody>
</table>

Figure 18. Tensile sample dimensions (in mm)
### TABLE V

Experimentally determined mechanical properties of aluminum 1100

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Yield Stress</td>
<td>90 MPa</td>
</tr>
<tr>
<td>Ultimate Tensile Strength (UTS)</td>
<td>120.0 MPa</td>
</tr>
<tr>
<td>Strain at UTS</td>
<td>0.048</td>
</tr>
<tr>
<td>Young Modulus</td>
<td>72.0 GPa</td>
</tr>
</tbody>
</table>

#### 6.3.2 Description of ultrasonic testing

Figure 21 shows the NLUT experimental setup. The transducers applied in this test were commercial piezoelectric transducers manufactured by Olympus Inc., with the effective diameter of 9.52 mm (0.375 in). The central frequencies of the transducers were 2.25 and 5 MHz as the transmitter and receiver, respectively. Figure 21(c) shows the calibration curves of transducers. The receiving transducer had a bandwidth in the range of 3.28-7.67 MHz such that the second and the third-harmonic frequencies could be measured. The transducers were placed facing to each other on the opposite sides of the specimen (Figure 21(a) and (b)), and light lubricant oil was applied between the surfaces as the couplant. The input signal was a 10-cycle, 100-Volt tone burst (i.e., harmonic signal with 10 cycles as shown in Figure 21(d)) at 2.25 MHz, which was generated by the Pocket UT system manufactured by MISTRAS Inc. The time-history signal of the 5 MHz receiver was recorded using the same UT system with the sampling frequency of 100 MHz and a band-pass filter of 1-20 MHz. Twenty signals were averaged to increase the signal to noise ratio (SNR).
6.3.3 Signal processing method to extract harmonic amplitudes

Figure 22 shows the wavelet-based signal decomposition method to calculate acoustic nonlinearity coefficients following the procedure described in Mostavi et al. (119). The first step in this method is to identify the harmonic frequencies of the received signal. These frequencies are visible in the frequency spectrum obtained by processing the measured time-domain signal with fast Fourier transform (FFT). As shown in Figure 22(a), the first harmonic frequency is near 2 MHz, the second-harmonic frequency is near 4 MHz and, the third-harmonic frequency is near 6 MHz. These frequencies are marked by three red lines on the wavelet spectrogram obtained by wavelet transformation (WT). The complex Morlet wavelet was implemented as the mother wavelet function. This mother wavelet is suitable for nonlinear ultrasonic testing, because it provides the best resolution in time and frequency, as well as precise

Figure 19. Stress-strain curves of samples with different strain levels
time localization. The spectral amplitudes over time, related to the red lines, are shown in Figure 22(c). The second- and third- order acoustic nonlinearity coefficients ($\beta$ and $\gamma$) were calculated over time using time-history signal of the harmonics and referring to Equation 3.22 and Equation 3.23 as shown in Figure 22(d). This procedure was repeated for each measurement and the average of $\beta$ and $\gamma$ over a specific time interval with constant plateau (in this research $3.0 \sim 4.0\mu s$) were calculated for each specimen. The measurements were performed along the gage length and shoulders of the specimens.

6.3.4 X-ray diffraction (XRD)

The X-ray diffraction technique was used to assess the plastic deformation in the materials with different strain levels and at two different locations, the shoulder of the tensile sample and at the center of the gage length for each strain. For this purpose, $15 \times 15mm$ samples were cut from the same place as the numerical model shown in Figure 23. The uniform and non-uniform plastic deformation was examined by full width at half maximum (FWHM) of XRD profile. XRD was carried out on a Siemens / Bruker D5000 X-ray Powder Diffraction (XRD) system with Cu-K radiation ($\lambda = 1.5418\AA$). The X-
Ray generator was run using a voltage of 40 KV and a current of 30 mA, with the samples scanned at 0.02°/step and 3s/step using a 2θ angle diffraction range from 30 to 80°.

### 6.4 Numerical modeling and results

In this section, the numerical simulation procedures and results of HOH generation in the aluminum specimen are presented.
Figure 22. Wavelet-based signal decomposition method to calculate acoustic nonlinearity coefficients, (a) FFT of the received signal, (b) spectrogram of the received signal, (c) the harmonic waveforms extracted from the wavelet transform and (d) the second and third acoustic nonlinearity coefficients

6.4.1 HOH changes at different positions of the specimen

Numerical simulation of NLUT was used to investigate the changes of HOH generation produced near the shoulder and the gage length of a dog-bone specimen. The specimen and its measurements shown in Figure 23 were modeled using Abaqus. To reduce the computation effort, only a quarter of the actual specimen was modeled and symmetric boundary conditions were imposed.
Experimental data obtained by tensile tests (Figure 18 and Table IV) along with isotropic hardening plasticity model described in Section 5.2 were used for the plasticity model. The model was first subjected to plastic deformation up to 4%. After the unloading stage, the ultrasound perturbation was introduced. The excitation area was modeled to generate the perturbation both on the shoulder and the gage according to Figure 23. After recording displacement histories from the area across from the excitation area, the acoustic nonlinearity parameter was calculated as described in Section 6.3.3. The waveforms and the frequency response for the gage and the shoulder for 4% plastic deformation are shown in Figure 24. Since the bandwidth of the fundamental frequency response from the numerical simulation is wide due to numerical resolution, it covers the second-harmonic’s frequency so that the second-harmonic cannot be observed explicitly. Nonetheless, for the nonlinearity calculations, it’s amplitude has been taken into account. The acoustic nonlinearity parameters based on the second and third-harmonic amplitudes for different strain levels are calculated and shown in Figure 25. In the middle of the specimen (gage), the third-harmonic acoustic nonlinearity coefficient ($\gamma$) increases up to 8%.
while the second-harmonic acoustic nonlinearity coefficient ($\beta$) increases up to 2%. Near the shoulder area, $\gamma$ increases up to 1130% and $\beta$ increases up to about 396%, both showing a clear upward trend.

In order to gain better insight into sources of HOH, two other numerical simulations were conducted. First the simulation is conducted for the shoulder part of the specimen and the linear elastic material model is assumed. No nonlinearity is inherent to the material model and the material is considered to be homogenous. The simulation result shows that although the geometrical variation exists in the model, no HOH is observed. It suggests that mere presence of the geometry variation does not contribute to the HOH, which could be artificially generated by the wave refraction/reflection within the geometric boundaries of non-uniform section. Secondly, the simulation is conducted for the middle part of the specimen and the $J_2$ plasticity model along with the experimental data is used for the material model. The simulation specimen is first subjected to plastic deformation up to 4%. After the unloading stage, a homogeneous plastic deformation is present in the model. The ultrasound perturbation is introduced afterward to analyze the HOH. No HOH generation was observed. It suggests that even though a plasticity model is used, mere homogeneous plasticity deformation does not significantly contribute to the nonlinearity of the model.

It is observed that as the distribution of plastic deformation gets non-uniform around shoulders, a better upward trend can be seen in $\beta$, while in both locations, $\gamma$ shows a higher sensitivity to deformation and can be a better indicator of nonlinearity within the specimen. The higher values of both nonlinearity indicators in shoulder areas of the dog-bone specimen are due to the non-uniformity of deformation as a result of geometry variation, which causes a higher plastic deformation and therefore excessive dislocation density in the mentioned areas (136). It is worth mentioning that in the shoulder area, mesoscale
heterogeneities do not have a major effect on the nonlinearity indicators since the geometrical variation provides large values of HOH. However, when monitoring the gage length of the specimen, since there is uniform strain distribution, mesoscale heterogeneities play an effective role in the nonlinearity of the material.

Figure 24. Time history waveforms and frequency responses for the gage and the shoulder at 4% plastic deformation

6.4.2 HOH changes due to heterogeneities

In this section, the mesoscale heterogeneities such as participates and second-phase particles, are considered in the model. To minimize the uniform-deformation condition induced by the geometry of the specimen, the gage part is chosen and modeled. The heterogeneous and elastoplastic material model used is described according to Section 5.2. To reduce the computational cost, only a fraction of the
The model was loaded up to strain levels of 1, 2, 3 and 4% and unloading, and then the ultrasonic excitation took place. The displacement history recorded on the receiving surface was used to calculate nonlinear acoustic nonlinearity coefficients. Figure 26 shows the calculated second- and third-harmonic acoustic nonlinearity parameters in heterogeneous media with respect to strain levels. As observed in Section 6.4.1, $\gamma$ is more sensitive than $\beta$. Increasing plastic deformation up to 4% leads to an increase of 28% in $\gamma$ while $\beta$ manifests a total of 6% increase in the plastic deformation of 4%, not showing a clear trend with the increase of plastic deformation.
6.5 **Experimental validation**

6.5.1 **NLUT results**

To characterize the effect of non-uniform plastic deformation on HOH, the shoulder area and gage area were experimentally studied. NLUT was performed three times at each location. Then, acoustic nonlinearity parameters were calculated as discussed in Section 6.3.3. Figure 28 shows the results of the NLUT measurements for the specimens subjected to different levels of plastic deformation. The points represent the mean value of the repeated measurements normalized by the pristine specimen, and the error bars represent the range of variation in the repeated measurements. Comparing the values

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1This sections results are courtesy of Amir Mostavi
of $\beta$ and $\gamma$, it is observable that $\gamma$ increases 2.8 times (780%) more than $\beta$ (275%) in the shoulder area. To characterize the effect of microscale heterogeneity on the second- and third-harmonic acoustic nonlinearity coefficients, NLUT was performed on the gage area where the deformation was uniform, and microstructure was heterogeneous. Comparing the values of $\beta$ and $\gamma$, it is observable that $\gamma$ increases 3.8 times (202%) more than $\beta$ (53%), which indicates a higher sensitivity of $\gamma$ to plastic deformation.

### 6.5.2 X-ray diffraction
Figure 28. Acoustic nonlinearity coefficients experimentally measured for the gage area and the shoulder area

X-ray diffraction (XRD) is one of the techniques used to measure the local strains and distinguish between uniform and non-uniform plastic deformations. The peak shift is usually associated with uniform strains and peak broadening is caused by non-uniform strains. This information on the plastic deformation in the material is due to changes in the crystal interplanar spacing and other lattice imperfections such as an increase in dislocation density. However, one major weakness of this method is its low penetration depth of the X-Ray beam, which is about 10 µm in most metals that makes the measurements only reliable at the surface of the material (137).

1This sections results are courtesy of Niloofar Tehrani
Figure 29 shows the full X-Ray diffraction pattern of the two samples, one from the center of the gage length and the other from the shoulder location of the specimen strained 2.5%. It is seen that all peaks shifted to higher $2\theta$ angles compared to the strain-free sample (according to standard XRD pattern for Aluminum, (PDF no. 04-0787), and this shift is larger in the shoulder compared to the center of the gage length. This indicates that the residual stresses are larger at the shoulder.

![Figure 29. XRD patterns of the 2.5% strain sample at two locations: gage and shoulder](image)

In assessing the gradual deformation produced by the systematic increments in strain, all samples were scanned near $2\theta = 78^\circ$. This range was selected since the inter-planar spacing of the high index planes are much smaller and any small fluctuations are easier to detect. Based on Bragg’s law ($\lambda = 2dsin\theta$), since $\lambda$ is constant for all the samples, there is a reverse relation between the $d$-spacing and
As the space between the planes decreases due to the previously applied tensile stress, $2\theta$ shifts to higher angles. Figure 30 shows such for all the samples at two locations. The displacements for the samples from the shoulder showed larger displacements as shown in Figure 31 as well as the increase in $2\theta$ displacement with higher strains. Note that the peak for the shoulder area strained to 4% the peak shifted to angles lower than $2\theta$ of the standard aluminum 1100 peak at this particular $2\theta$ angle. This can be due to the fact that at this strain level, the tension and compression stresses are both present because of the non-rectangular shape and drastic geometric change of the specimen from shoulder to gage length. In this case, the compression strains may have become dominant and shift the peak to lower $2\theta$ values. In addition, although the samples are all from the same plate, the rolling might not be uniform, and the machining of the specimen might leave residual stresses that already can affect the crystals $d$-spacing for each sample before any applied strain.

As mentioned earlier, the XRD test only monitors the surface of the material. A numerical test is conducted to further support the XRD results. The above numerical simulations are carried out, this time considering only the surface layer elements in the model. The maximum of through-thickness strain ($\epsilon_{33}$) is measured on the surface layer for strains up to 4%. As the strain is increased in the loading stage, the remaining compressive strains through the specimen are also increased. The maximum through-thickness strain on the surface layer has a positive sign when the plastic deformation is increased from 0 to 3% with a tendency to decrease in value. However, at 4% strain, the sign of $\epsilon_{33}$ changes to a negative value. The $\epsilon_{33}$ values are shown in Figure 32. This result is in line with the XRD results that show the dominance of the compression strains in the 4% samples due to the irregular geometry and therefore the non-uniform deformation. However, when analyzing the gage length, the tensile test accompanied
Figure 30. XRD patterns of all the samples at about $2\theta = 78^\circ$ for (a) gage, and (b) shoulder by Poisson’s effect introduces compressive through-thickness uniform strains from the very beginning. The deformation is uniform and therefore there is no tensile strain $\epsilon_{33}$ present in the sample. The compressive strain value increases as the tension increases throughout the sample.

Figure 33 shows the results of the line broadening effects. As indicated earlier, line broadening in X-Ray peaks is associated with non-uniform strains, which in this investigation is primarily expected in the shoulders of the tensile specimen caused by the geometrical changes due to the transition from the grip areas into the gage length. The line broadening was calculated using full width at half maximum (FWHM). FWHM can be used to determine the relative non-uniform plastic deformation. As the amount of non-uniform plastic deformation increases, the broadening in the peaks increases. In the cases that the
uniform and non-uniform plastic deformations are both present, a mixture of peak shift and broadening can be observed. Based on the observations in Figure 33, the FWHM for the shoulder area is higher than the gage area for each sample at different strain levels, except at the strain level 0.15, which indicates higher non-uniform plastic deformation in this region due to the significant geometrical changes. The small increases in line broadening observed for the samples extracted from the gage length (15%) is further evidence that a uniform straining occurs at the gage location. On the other hand, the shoulder sample shows an 83% increase in FWHM from 0.5% to 4% strain. This high increase in broadening re-confirms the presence of non-uniform plastic deformation in the shoulder compared to the gage length.
6.6 Discussions

To investigate the effect of non-uniform plastic deformation due to the geometry of the specimen, the acoustic nonlinearity parameters are measured at different locations of dog-bone specimens. As the nonlinearity is measured near the shoulder, the numerical analysis shows up to 1130% increase in the third-harmonic acoustic nonlinearity coefficient ($\gamma$), while the second-harmonic acoustic nonlinearity coefficient ($\beta$) shows up to about 396% increase. On the other hand, measuring the nonlinearity parameters near the shoulder experimentally shows about 780% increase in $\gamma$, while this increase is about 275% for $\beta$. In both numerical and experimental studies, $\gamma$ is approximately 2.8 times more sensitive than $\beta$ in the shoulder part of the specimen. On the other hand, when the deformation in macroscale is considered uniform in the middle of the specimen, numerical analysis shows up to 8% increase in $\gamma$. 

Figure 32. The maximum through-thickness strain in the surface layer of shoulder part measured numerically
Figure 33. FWHM of the samples with different strain levels at \(2\theta \approx 78^\circ\)

while this increase is about 2% for \(\beta\) with no clear trend. Experiments show an increase of 200% in \(\gamma\) and 53% in \(\beta\), confirming the higher sensitivity of \(\gamma\).

Considering the mesoscale heterogeneity, numerical analyses indicate that the mesostructural variations distort the ultrasound waveform, stimulating \(\gamma\) increase up to 30%, however \(\beta\) does not show a clear trend when plastic deformation increases.

Series of XRD tests are carried to observe the non-uniform plastic deformation effect in microscale. Observing the microstructural level, line broadening in XRD results expresses the fact that the deformation is non-uniform in the irregular geometry of the shoulder area compared to the gage section. The non-uniformity of stress results in localized plastic deformation and contributes to the higher nonlinearity of the material in the shoulder area which can be assessed with the HOH generations.
6.7 Conclusions

The source of nonlinearity in materials can be attributed to many physical phenomena. In this study, the subject of generating HOH in ultrasonic waves due to non-uniform deformation produced by different scales of irregularities under plastic deformation has been investigated numerically and experimentally. Understanding the correlation between non-uniform plastic deformation and HOH generation provides a quantitative method to assess the nonlinearity and therefore damage in structures and predict the eventual fracture. For this purpose, different length scales of material have been considered for the nonlinearity characterization.

To understand the correlation between meso- and macro-scale irregularities and material nonlinearity, the HOH acoustic nonlinearity coefficients need to be measured under different plastic deformations. When a specimen is under plastic deformation, the non-uniform plastic deformation is generated in the areas with meso- and macro-structural variations, which distort the ultrasound waveform.

Both numerical and experimental studies confirm that non-uniform plastic deformation increases HOH, whether the non-uniformity is due to microscale heterogeneity or macroscale variations. XRD studied on the microstructure of the samples reveals the effect of macroscale variations on the microstructure of the material, providing an extra magnified insight into the material nonlinearity and their sources. In addition, the third-harmonic acoustic nonlinearity coefficient proves to be a more sensitive indicator of the material nonlinearity in dealing with microstructural heterogeneity or geometric variations in the structure.

This study provides an insight of the sources of nonlinearity in materials with different scales of structural irregularities. Future analysis of the contribution of different nonlinearity stimulators in HOH
generation can lead to a more thorough understanding of NLUT and better interpreting its results. Having a clear understanding of the nonlinearity sources can deliver more accurate experimental results by eliminating external and unwanted factors that contribute to HOH. Moreover, higher sensitivity of the third-harmonic acoustic nonlinearity coefficient under the presence of non-uniform deformation can be explored further in other materials such as composite, steel etc.
CHAPTER 7

ENRICHED FINITE ELEMENT METHOD FOR NONLINEAR ACOUSTICS

Computational acoustics has been an area of active research for almost half a century. It also has been applied to other fields, such as geophysics, meteorology, electromagnetics, etc. In particular, the challenge of efficient computation at high wave numbers is one of the problems still unresolved by current numerical methods. Standard FE methods are inherently demanding while tackling problems with high wave numbers because they require an excessive computational effort in order to resolve the waves and control numerical dispersion errors. The deficiency to a decent representation of sub-mesh scales not only misses the fine-scale part of the solution, but often causes the so-called numerical dissipation and dispersion errors in the solution on the resolved scale as well. This phenomenon is related to the deterioration of numerical stability due to accumulation of dispersion error. In order to cope with such error effectively, many current discretization techniques are being developed. In this chapter, an enriched numerical method is discussed and some benchmark problems are solved. To solve for nonlinear wave propagation problems, a user element (UEL) with enriched FE characteristics is developed in Abaqus™, and the results are discussed.

7.1 Formulation of the method

As described in the previous chapter, consider the governing continuum mechanics equations for the body $\Omega$ are derived as below.
In this boundary value problem, the body of interest \( \Omega \) has a boundary \( \Gamma \) with the displacement specified on Dirichlet boundary (\( \Gamma_D \))

\[
\mathbf{u} = \mathbf{u}_D
\]  

(7.2)

and on Neumann boundary \( \Gamma_N \), tractions are specified,

\[
\sigma(\mathbf{u}).\mathbf{n} = h
\]  

(7.3)
where \( h \) is the imposed boundary traction vector, \( n \) is the outward unit normal and \( b \) represents the body force acting on \( \Omega \).

Taking the strong form of the differential equation, multiplying by a test function will result in the variational form of the governing continuum mechanics equations:

\[
\int_{\Omega} \rho \delta u \frac{\partial^2 u}{\partial t^2} d\Omega = \int_{\Omega} \delta u \nabla \cdot \sigma d\Omega + \int_{\Omega} \delta u \cdot b d\Omega \quad (7.4)
\]

after integration by parts and the divergence theorem, we have:

\[
\int_{\Omega} \nabla \delta u : \sigma d\Omega + \int_{\Omega} \rho \delta u \frac{\partial^2 u}{\partial t^2} d\Omega = \int_{\Gamma_N} \delta u \cdot h d\Gamma + \int_{\Omega} \delta u \cdot b d\Omega \quad (7.5)
\]

we approximate the variational form with the Galerkin weak formulation as:

\[
\int_{\Omega} \nabla \delta u : \sigma^h d\Omega + \int_{\Omega} \rho \delta u \frac{\partial^2 u}{\partial t^2} d\Omega = \int_{\Gamma_N} \delta u \cdot h d\Gamma + \int_{\Omega} \delta u \cdot b d\Omega \quad (7.6)
\]

Equation 7.6 will be discretized in space which leads to the matrix form as presented below:

\[
\begin{bmatrix} M \end{bmatrix} \ddot{U} + \begin{bmatrix} K \end{bmatrix} U = R \quad (7.7)
\]

where \( M \) and \( K \) are mass and stiffness matrices and \( U \) and \( R \) are nodal displacements and externally applied forces respectively.
7.1.1 Spatial discretization

While we consider one and two-dimensional analysis of solids, the basic equations can directly be generalized to multi-dimensional solutions. Considering only one typical solution variable \( u \) the element interpolation functions or shape functions for Equation 7.5 for two-dimensional analyses are given by (27):

\[
\begin{align*}
\mathbf{u}(\xi, \eta) &= \sum_{i} N_P \mathbf{h}_i(\xi, \eta) [U(I_0, 0, 0) + \sum_{j} \left\{ \sin\left(\frac{\pi j}{2h_x} x\right)U^s_{(I,j,0)} + \cos\left(\frac{\pi j}{2h_y} y\right)U^c_{(I,j,0)} \right\}] + \\
&\sum_{l} \left\{ \sin\left(\frac{\pi l}{2h_y} y\right)U^s_{(I,0,l)} + \cos\left(\frac{\pi l}{2h_y} y\right)U^c_{(I,0,l)} \right\} + \\
&\sum_{j} \sum_{l} \left\{ \sin\left(\frac{\pi j}{2h_x} x + \frac{\pi l}{2h_y} y\right)U^{s+}_{(I,j,l)} + \cos\left(\frac{\pi j}{2h_x} x + \frac{\pi l}{2h_y} y\right)U^{c+}_{(I,j,l)} \right\} + \\
&\sum_{j} \sum_{l} \left\{ \sin\left(\frac{\pi j}{2h_x} x - \frac{\pi l}{2h_y} y\right)U^{s-}_{(I,j,l)} + \cos\left(\frac{\pi j}{2h_x} x - \frac{\pi l}{2h_y} y\right)U^{c-}_{(I,j,l)} \right\}
\end{align*}
\]

(7.8)

where \( \mathbf{U} \) with superscripts are the nodal degrees of freedom. \( NP \) is the number of shape functions in each element, \( m \) and \( k \) are number of sin and cos functions, respectively, considered. \( 2j \) and \( 2l \) are the number of cycles of harmonic functions within one element which are called “the cutoff numbers”.

In this approach, the conventional interpolation functions are enriched by harmonic functions and interpolation used for displacements are obtained. We use \( N_I \) in the natural space \( \xi \) and \( \eta \). In Equation 7.8 \( h_x \) and \( h_y \) are the typical element sizes is \( x \) and \( y \) directions. In particular, in our numerical technique, fundamental frequency of the enrichment functions has been chosen such that an integer number of harmonics are within one element.
This particular interpolation function is chosen on purpose to benefit from its applicability and accuracy in solving ultrasonic wave propagation problems. The advantages include the fact that we already know the fundamental frequency range in UT and moreover, second harmonic’s frequency is also known which is twice the fundamental frequency. Therefore, with those known harmonics embedded in the solution space, more accurate solutions can be obtained.

7.1.2 Boundary conditions

Due to the enrichment function in Equation 7.8, the Kronecker delta properties existing in the conventional finite element may not be guaranteed after the enrichment. To overcome the issue while maintaining optimal convergence. Nitsche’s method is introduced to impose essential boundary conditions. Nitsche’s approach is a scheme to overcome the (possible) accuracy deficiency on boundaries. There are other methods like penalty method or Lagrange-multiplier methods. The traditional way of imposing Dirichlet boundary conditions can be problematic. Nitsche discusses techniques for incorporating Dirichlet boundary conditions in the weak form of the model problem. Let’s consider the Poisson’s problem:

\[-\Delta u = f \quad \text{in} \quad \Omega \quad \quad \text{(7.9)}\]

\[u = g \quad \text{on} \quad \Gamma = \partial \Omega \quad \quad \text{(7.10)}\]
multiplying the strong form by a test function, we obtain

\begin{align}
\int_{\Omega} f w d\Omega &= -\int_{\Omega} \Delta u w = \int_{\Omega} \nabla u \cdot \nabla w d\Omega - \int_{\partial\Omega} \nabla u \cdot n w ds = \\
\int_{\Omega} \nabla u \cdot \nabla w d\Omega - &\int_{\partial\Omega} \nabla u \cdot n w ds - \int_{\partial\Omega} (u - g) \nabla w \cdot n ds
\end{align}

(7.11)

where in the last part \( u - g = 0 \) has been added. Rearranging the terms to linear and bilinear parts, another term \( \eta \int_{\partial\Omega} (u - g) w ds \) is added for sufficiently large \( \eta > 0 \) to ensure coercivity.

\begin{align}
\int_{\Omega} \nabla u \nabla w d\Omega - &\int_{\partial\Omega} \nabla u \cdot n w ds - \int_{\partial\Omega} u \nabla w \cdot n ds + \eta \int_{\partial\Omega} u w ds = \\
- \int_{\partial\Omega} g \nabla w \cdot n ds + &\eta \int_{\partial\Omega} g w ds + \int_{\Omega} f w d\Omega
\end{align}

(7.12)

### 7.2 One dimensional problem

In this part, the performance of enriched FE is assessed by solving a one dimensional transient wave propagation problem.

#### 7.2.1 numerical example and results

The problem considered is dynamic analysis of a one dimensional bar with length \( L \) and Young modulus of \( E \) with enriched FE method. For this problem, the solution of \( u \) is governed by

\[ \frac{\partial^2 u}{\partial t^2} - c^2 \frac{\partial^2 u}{\partial x^2} = 0 \]

(7.13)

with the boundary conditions:

\[ u(0,t) = 0 \]

(7.14)
\[ \frac{\partial u}{\partial x}(L, t) = u_0 \frac{\pi E}{L} \sin(c_l \frac{\pi}{L} t) + u_1 \frac{2\pi E}{L} \sin(c_l \frac{2\pi}{L} t) \] (7.15)

And initial conditions:

\[ u(x, 0) = 0 \] (7.16)

\[ \frac{\partial u}{\partial t}(x, 0) = -u_0 c_l \frac{\pi}{L} \sin \frac{\pi}{L} x + u_1 c_l \frac{2\pi}{L} \sin \frac{2\pi}{L} x \] (7.17)

the analytical solution of this problem has the following expression:

\[ u = u_0 \sin \frac{\pi}{L} x \sin \left(c_l \frac{\pi}{L} t\right) + u_1 \sin \frac{2\pi E}{L} x \sin \left(c_l \frac{2\pi}{L} t\right) \] (7.18)

In Figure 35 the exact solution of \( u \) alongside both FE method and enriched FE method is illustrated and the absolute difference error value \( e_h = u(x) - u_h(x) \) is calculated using equal sized elements in each solutions. The error in FE solution is due to wavelength elongation and amplitude decay known as numerical dispersion and dissipation error.

It is clearly observable that FE method with 60 elements and 61 degrees of freedom has an accuracy in the order of \( 10^{-3} \) while enriched FE is capable to maintain the accuracy in order of \( 10^{-4} \) with only 8 elements and 45 degrees of freedom (cutoff number =2).

Incorporating Nitsche’s approach on imposing boundaries, the results are as below:
Comparing the error from imposing the boundary condition directly and by Nitsche’s method, it can be clearly observed that the latter enhances the accuracy of the solution by almost 100 times.

### 7.3 Two dimensional problems

In this section, we illustrate the performance of the enriched finite element method by solving time harmonic transient scalar wave problems and the results are discussed.
7.3.1 Problem statement

The scalar wave equation with a Ricker wavelet source at the center of a two dimensional domain is modeled.

\[
\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + F(0, 0, t) = \frac{1}{c^2} \frac{\partial^2 u}{\partial t^2}
\]  
(7.19)

\[
F(0, 0, t) = 10(1 - 2\pi^2 f^2(t - 0.25)^2) \exp(-\pi^2 f^2(t - 0.25)^2)
\]  
(7.20)

where \(u\) is the displacement solution, \(c\) is the wave velocity (in this example \(c = 1\)), \(f\) is the central frequency, (in this example \(f = 6Hz\)). Due to symmetry, only a quarter of the area is used for FE solution which is a \([0, 1] \times [0, 1]\) domain. Generally, in dealing with wave propagation problems, absorbing boundary conditions are used, however, here for the time considered 0.95s, the wave does not
get to the boundary, hence there will be no reflections and no need for the absorbing boundary conditions. Quadratic elements are used both for standard FE and enriched FE solutions. The FE model has been discretized with 60 by 60 mesh leading to 3721 degrees of freedom while enriched FE model is discretized by $8 \times 8$ mesh with cutoff numbers $(k,m) = (1,1)$ leading to 729 degrees of freedom.

In both models, trapezoidal rule of time integration is used with time step size $\delta t = 0.00625$

7.3.2 Results

The snapshots of results are given at time $0.95s$. As expected, the numerical solution of the enriched model shows better accuracy, while using less time and space in the machine memory.
7.4 Nonlinear enriched FEM

As discussed in the previous chapters, nonlinear ultrasonic methods have strong potential to identify damage and flaws in materials, hence increasing the possibility of correctly predicting the remaining life of structures. In previous section, the capability and accuracy of an enriched FE method was discussed. In this section, enriched FE method is applied to solve for nonlinear wave propagation, aiming to obtain
an efficient yet accurate waveform results. To this end, a User Element (UEL) script is written and incorporated in to the Abaqus™ finite element code.

User subroutines can be written in Fortran or C-codes. With UEL subroutine, a maximum of 30 degrees of freedom becomes possible. The main objective of a user element is to provide Abaqus™ solver with the stiffness matrix and the residual vector, which is in line with the context of solving a nonlinear system of equation using a Newton-Raphson method. At the end of this section, the simulation results are demonstrated and compared with Abaqus™ standard elements.

7.4.1 An enriched FE user element framework

The enriched FE subroutine is written with Fortran code. In this subroutine, 10 degrees of freedom per each node is used, reach of which represent different displacement enrichments demonstrated in Equation 7.8. As discussed before, in order to solve the nonlinear system of equations, the right hand side (residual) vector and the tangent (stiffness) matrix are needed. Following equations are resumed after the weak form of the momentum balance Equation 7.5 which in general, requires the application of an iterative solution scheme such as Newton-Raphson. Considering this, the system of equations have to be linearized. Consequently, \( F^N \) is defined as a residual quantity by:

\[
F^N = F^N_{ext} - F^N_{int}
\]  

(7.21)

in which \( F^N_{ext} \) is the external nodal forces (depending on the problem, can be moments, heat flow, etc.) due to applied loads and \( F^N_{int} \) is the internal nodal forces (due to stress, etc.) at node N and they depend on the values at nodal degree of freedom \( u^N \) at node N.
Another requirement of solving the iterative nonlinear system of equations is to define the stiffness matrix (Jacobian):

\[ K^{NM} = -\frac{dF^N}{du^M} \] (7.22)

In the case of dynamic analysis, the forces and the Jacobian are specified and correspond to the integration procedure used as:

\[ F^N = -M^{NM}u_{t+\Delta t}^M + (1 + \alpha)G_{t+\Delta t}^N - \alpha G_t^N \] (7.23)

\[ K^{NM} = -M^{NM}\left(\frac{1}{\beta \Delta t^2}\right) + (1 + \alpha)K_s^{NM} \] (7.24)

neglecting the damping in the model. In the above equations, \( K_s^{NM} \) is the static tangent stiffness matrix, \( \beta = (1/4)(1 - \alpha^2) \) is the Newmark-\( \beta \) operator, \( \alpha \) is the Hughes-Hilbert-Taylor integration operator. For simplicity \( \alpha \) is set to zero and \( \beta \) and \( \gamma \) are 0.25 and 0.5 to simulate the trapezoidal rule of integration.

In general, a summary of the procedure utilizing the user subroutine can be viewed in the following flow chart:
Initialize

Start of analysis

Start of increment

Define Initial Conditions

Calculate Integration Point Field Variable from Nodal Values

Start of Iteration

Calculate $\Delta \epsilon$

Calculate $\sigma$, $\frac{\partial \Delta \sigma}{\partial \Delta \epsilon}$

Define Loads $\mathbf{R}$

Solve $\mathbf{Ku} = \mathbf{R}$

Converged?

yes

no

End of step?

yes

Write Output

no

Figure 39. Flow Chart
7.4.2 Numerical example

The enriched FEM is tested for a nonlinear wave propagation problem against Abaqus standard elements. The Neo-Hookean model with parameters $C_{10} = 1325 \text{ GPa}$ and $D_1 = 2.89E-005 \text{ GPa}^{-1}$ are employed as hyperelastic material. For the enriched FE, 8 additional degrees of freedom are used. The configuration of the problem is depicted as below:

![Figure 40. Two dimensional model used to test enriched FE](image)

A sine wave is applied uniformly at one edge and the results are measured at the nodes on the edge across from it and then averaged. The following figure demonstrates the results of both enriched FE and standard FE with different element numbers:

In the enriched FE solution there are 39 elements and 800 degrees of freedom used and for the standard FE two models with 1500 elements and 6000 degrees of freedom and 75 elements and 152 degrees of freedom are used. The accuracy of enriched FE with only 39 elements is comparable to the converged standard FE model with 1500 elements. 1500 elements are required to provide the maximum element size used allowed for nonlinear wave propagation analysis. The computational efficiency for both time and space of the enriched FE algorithm is higher than standard FE. The time used for enriched
Figure 41. A nonlinear wave analyzed by different Enriched and Standard FE

FE analysis is one fourth of the standard FE analysis time and the memory used in the enriched FE is also almost one fourth. The results clearly show the accuracy as well as the efficiency of enriched FE with respect to the standard FE model.

7.5 Conclusions

In this chapter, different linear and nonlinear wave propagation problems are discussed and compared with standard FE solutions. For both cases, it is observed that when conventional FE interpolation functions are enriched with the specific solution of the problem, a more accurate yet efficient solution can be obtained.
CHAPTER 8

HARMONIC-ENRICHED RKPM FOR WAVE PROPAGATION PROBLEMS

In this chapter an implicit enrichment scheme based on reproducing kernel particle method (RKPM) to effectively solve high frequency wave propagation problems is presented. The characteristic function are embedded in the basis function for constructing RK approximation. This approach allows better solution accuracy without adding to the degrees of freedom. As a result, the high frequency wave problem can be solved using less nodes, enhancing both computational efficiency and accuracy. Application of this techniques is particularly useful for the numerical simulation of ultrasonic testing (UT) of structures due to the high frequency of the utilized transducer. Specially in numerical simulation of nonlinear UT when higher harmonics are sought in the received wave response, and the traditional FE needs to have a very fine mesh to produce desirable results, employing this technique shows to be even more functional. The proposed method is assessed through von Neumann analyses and verified with several numerical examples.

8.1 Introduction

A thorough literature review of the enhanced numerical methods (Spectral methods, Partition of unity methods, element free methods, etc.) for solving wave propagation problems and the challenges for accurate and efficient simulations are given in Section 2.4. In numerical modeling of nonlinear ultrasonic testing (NLUT), as looking for the second harmonic and, in the heterogeneous material cases, the third harmonic, the mesh size is required to be very small. Decreasing mesh size will in turn cause
dispersion and dissipation problems while increasing the computational effort to the extent that the numerical modeling requires excessive effort.

In this chapter, tackling the issue of computational efficiency in high frequency wave propagation problems using harmonic basis functions to implicitly enrich RKPM is discussed. This technique enables the solution to take advantage of both element free and spectral methods without adding to the degrees of freedom.

The organization of this chapter is as follows. In 8.2, the interpolation scheme in RKPM method and governing equation is reviewed and the newly developed H-RKPM is proposed. In 8.3, the dispersion and stability analysis of H-RKPM is calculated and compared with the standard RKPM and FE. In 8.4, one dimensional and two dimensional numerical examples are solved to illustrate the performance of implicit enrichment. In 8.5, remarks are provided to conclude the paper.

8.2 Theory and implementation

In this section, a brief overview of the RKPM method is presented and the implicit enrichment of RKPM for solving wave propagation problems is introduced.

8.2.1 RK approximation

As described in the Section 8.1, the development of interpolation functions in computational methods in an attempt to approximate the solution field $u(x)$ is the ultimate target of many computational methods. Consider a close domain $\Omega$ discretized by a set of $NP$ points. The RK approximation function is as below:

$$u(x) \approx u_h(x) = \sum_{I=1}^{NP} \Psi_I(x) u_I$$  (8.1)
where $\Psi_I$ represents the RK shape function and $u_I$ is the corresponding nodal coefficients.

$$
\Psi_I(x) = \phi(x)[a_I + b_{IJ}f_j(x)] \tag{8.2}
$$

The RK shape functions are constructed by two main functions, a kernel function $\phi_a$ and a correction function $C$.

$$
\Psi_I(x) = C(x; x - x_I)\phi_a(x - x_I) \tag{8.3}
$$

where kernel function is defined on a bounded space centered at $x_I$ and $a$ is the radius (support domain size) of the kernel function. Kernel determines the smoothness (order of continuity) and locality of shape functions. Usually, B-splines of different orders are used as the kernel functions. The most common kernel used for constructing RK shape functions is cubic B-spline which provides $C^2$ continuity.

On the other hand, the correction function $C(x; x - x_I)$ is introduced for obtaining monomial reproducitity below,

$$
\sum_{I=1}^{NP} \Psi_I(x - x_I)x_1^i x_2^j x_3^k = x_1^i x_2^j x_3^k \tag{8.4}
$$

where $i + j + k = 0, 1, \ldots, n$. $n$ is the highest order of complete monomials.

The correction function is introduced in the form below,

$$
C(x; x - x_I) = H^T(x - x_I)b(x) \tag{8.5}
$$
where \( H^T(x - x_I) \) is the basis vector shown in Equation 8.6 and \( b(x) \) is the coefficient vector which is obtained in Equation 8.7 by introducing Equation 8.5 into Equation 8.4.

\[
H^T(x - x_I) = [1 \ x_1 - x_{1I} \ x_2 - x_{2I} \ \cdots \ (x_3 - x_{3I})^n]
\]  

(8.6)

\[
b(x) = M^{-1}(x)H(0)
\]  

(8.7)

where \( M(x) \) is called the moment matrix, which plays an important role in constructing RK shape functions. A required minimum number of points are needed for constructing moment matrix such that it is invertible. Moment matrix is in form of Equation 8.8

\[
M(x) = \sum_{I=1}^{NP} H(x - x_I)H^T(x - x_I)\phi_a(x - x_I)
\]  

(8.8)

Finally, by substituting Equation 8.7 into Equation 8.5 and then Equation 8.1, RK shape function is obtained as,

\[
\Psi_I(x) = H^T(0)M^{-1}(x)H(x - x_I)\phi_a(x - x_I)
\]  

(8.9)

### 8.2.2 Harmonic-enriched reproducing kernel formulation

As discussed in the previous section, in conventional way of constructing RK shape functions, correction function \( C(x; x - x_I) \) is introduced such that monomial reproductivity are obtained, as shown in Equation (Equation 8.4). For this purpose, components of basis vector \( H(x - x_I) \) are selected as a set of complete polynomial terms up to the desired order \( n \). Although polynomial-based RK shape functions provide algebraic error convergence rate, obtaining promising accuracy for non-polynomial functions
approximation and also PDE solutions may need considerably fine discretization (or high number of source points in mesh-free methods) to obtaining a desirable level of accuracy. Even though increasing the nodes/points in both methods can help to overcome this issue to some level, computational efficiency and machine’s memory management still remain as main challenges. Using explicit enrichment in the FEM framework is shown to relax the oscillations [27], however increasing the number of degrees of freedom (DOFs) could be still recognized as a computational efficiency issue.

To address discussed issues above, in this work, basis vector used in the correction function is proposed to be chosen such that it satisfies the trigonometric (harmonic) reproducing conditions. The idea comes from the fact that wave propagation problems have harmonic behavior in nature. Satisfying trigonometric reproducing conditions enhances accuracy of the function approximation and also approximating the solution of the wave propagation problems. With the same idea as in polynomial-based RK shape functions where the terms of Taylor expansion is used, for harmonic-enriched RK, the terms of Fourier (trigonometric) series could be chosen as the basis-vector’s terms.

A trigonometric (Fourier) is the expansion of periodic function in terms of \( \sin \) and \( \cos \), making use of the orthogonality property of the harmonic functions. Considering a single-valued function \( f(\omega x) \). The trigonometric expansion of \( f(\omega x) \) is written as in \( \text{Equation 8.10} \),

\[
f(\omega x) = \frac{1}{2}a_0 + \sum_{k=1}^{\infty} a_k \cos(\omega k x) + \sum_{k=1}^{\infty} b_k \sin(\omega k x)
\]

(8.10)

A complete trigonometric basis terms of order \( m \) for the Fourier series are all the term including \textit{sines} and \textit{cosines} for \( k = 0, \cdots, m \) and a constant term. With the same approach as extracting monomial
basis terms from Taylor expansion, by ignoring the coefficients of the Fourier series, the harmonic basis vector $H(x)$ of order $m$ for one-dimensional case could be written as,

$$H^T(x) = [1, \sin(\omega x), \cos(\omega x), \cdots, \sin(m\omega x), \cos(m\omega x)]$$

(8.11)

By definition of Fourier series, for a periodic function $f(\omega x)$ with continuous first and second derivatives, it is guaranteed that the trigonometric series of $f(\omega x)$ converges uniformly to $f(\omega x)$ for all $x$, also known as Dirichlet conditions. In other words, by selecting adequate complete terms of the Fourier series as the components of the basis order, more accurate numerical results are expected when approximating function.

However, including more terms in the basis vector results in a larger basis vector and consequently a larger moment matrix $M$ and an increase in its condition number. All these result in an increase in the computational cost and also a decrease in accuracy of the numerical solution.

To address both CPU-time and accuracy issues, in this paper, the idea of harmonic based RK shape functions is proposed by choosing the basis vector terms’ frequency, same as the characteristics available or the excitation frequency of the problem. For instance, assuming analytical solution of a wave propagation problem as in Equation 8.12,

$$u(x) = A \sin(\omega_1 x) \sin(\omega_2 t) + B \cos(\omega_1 x) \cos(\omega_2 t)$$

(8.12)

The basis vector could be constructed as $H(x) = [1, \sin(\omega_1 x), \cos(\omega_1 x)]$ including sin and cos of arguments shown in the equation (here $\omega_1 x$). It will be shown in the following that for harmonic
reproducing conditions, a set of complete trigonometric terms must be chosen in the basis vector. By
definition, a complete set of trigonometric terms are those which can satisfy the partition of unity (con-
stant term in Fourier series) and reproducing condition for all terms included in the basis vector. For the
cases which analytical solution is not provided, excitation frequency is observed to be used for acquiring
the most accurate solution.

An expansion by a complete set of functions can be easily generalized for higher dimensions, as well.

Assuming a two-dimensional function of \( f(\omega_1 x, \omega_2 y) \), formed of an orthonormal complete system of
functions \( \cos(\omega_1 x) \cos(\omega_2 y), \sin(\omega_1 x) \cos(\omega_2 y), \cos(\omega_1 x) \sin(\omega_2 y), \) and \( \sin(\omega_1 x) \sin(\omega_2 y) \) expansion
of \( f(\omega_1 x, \omega_2 y) \) can be written as,

\[
f(\omega_1 x, \omega_2 y) = \sum_{k=1}^{\infty} \sum_{l=1}^{\infty} \lambda_{kl} \left\{ a_{kl} \cos(\omega_1 kx) \cos(\omega_2 ly) \\
+ b_{kl} \sin(\omega_1 kx) \sin(\omega_2 ly) + c_{kl} \cos(\omega_1 kx) \sin(\omega_2 ly) \\
d_{kl} \sin(\omega_1 kx) \sin(\omega_2 ly) \right\}
\] (8.13)

For both one and two dimensional cases, basis vector’s terms must be selected such that the shifted
reproducing conditions are obtained. For instance, for one-dimensional case with trigonometric terms,
it can be shown that both \( \sin(\omega_1 x) \) and \( \cos(\omega_1 x) \) must be included in the basis vector for satisfying the
reproducing conditions. Defining the harmonic-enriched RK shape-function as,

\[
\Psi_I(x) = C(x; x - x_I) \phi_0(x - x_I)
\] (8.14)
Considering the first order trigonometric terms for one-dimensional case, correction function \( C \) can be written as,

\[
C(x; x - x_I) = b_0(x) + b_1(x) \sin \omega(x - x_I) + b_2(x) \cos \omega(x - x_I)
\]

\[=: \mathbf{H}^T(x - x_I)\mathbf{b}(x),\]

where the coefficients \( b_i(x), (i = 0, 1, 2) \) are determined by satisfying the partition of unity and reproducing conditions for harmonic terms shown below,

\[
\sum_{I=1}^{NP} \Psi_I(x) = 1 \quad (8.16a)
\]

\[
\sum_{I=1}^{NP} \Psi_I(x) \sin(x_I) = \sin(x) \quad (8.16b)
\]

\[
\sum_{I=1}^{NP} \Psi_I(x) \cos(x_I) = \cos(x) \quad (8.16c)
\]

For showing the shifted reproducing conditions, from \( \text{Equation 8.16} \), multiplying \( \text{Equation 8.16b} \) by \( \cos(x) \) and \( \text{Equation 8.16c} \) by \( \sin(x) \) can show,

\[
\sum_{I=1}^{NP} \Psi_I(x) \sin(x_I) \cos(x) = \sin(x) \cos(x) \quad (8.17a)
\]

\[
\sum_{I=1}^{NP} \Psi_I(x) \sin(x) \cos(x_I) = \cos(x) \sin(x) \quad (8.17b)
\]
By subtracting (Equation 8.17b) from (Equation 8.17a),

\[ \sum_{I=1}^{NP} \Psi_I(x)[\sin(x_I) \cos(x) - \sin(x) \cos(x_I)] = \sum_{I=1}^{NP} \Psi_I(x) \sin(x - x_I) = 0 \quad (8.18) \]

Similarly, multiplying (Equation 8.16b) by \( \sin(x) \) (Equation 8.16c) by \( \cos(x) \),

\[ \sum_{I=1}^{NP} \Psi_I(x) \sin(x_I) \sin(x) = \sin^2(x) \quad (8.19a) \]
\[ \sum_{I=1}^{NP} \Psi_I(x) \cos(x) \cos(x_I) = \cos^2(x) \quad (8.19b) \]

Summation of (Equation 8.19a) and (Equation 8.19a),

\[ \sum_{I=1}^{NP} \Psi_I(x)[\sin(x_I) \sin(x) + \cos(x) \cos(x_I)] = \sum_{I=1}^{NP} \Psi_I(x) \cos(x - x_I) = 1 \quad (8.20) \]

Eventually, the partition of unity and shifted harmonic reproducing conditions can be equivalently written as,

\[ \sum_{I=1}^{NP} \Psi_I(x) = 1 \quad (8.21a) \]
\[ \sum_{I=1}^{NP} \Psi_I(x) \sin(x - x_I) = 0 \quad (8.21b) \]
\[ \sum_{I=1}^{NP} \Psi_I(x) \cos(x - x_I) = 1 \quad (8.21c) \]
where we can eventually express the reproducing conditions as,

$$\sum_{I=1}^{NP} \Psi_I(x)H(x - x_I) = H(0), \quad H^T(0) = [1, 0, 1]$$ \hspace{1cm} (8.22)

Substituting \textit{(Equation 8.14)} and \textit{(Equation 8.15)} into \textit{(Equation 8.22)},

$$M(x)b(x) = H(0)$$ \hspace{1cm} (8.23)

where $M(x)$ is the moment matrix constructed using newly-proposed harmonic basis vector $H(x - x_I)$. Consequently, harmonic-enriched RK shape-functions could be constructed same as the polynomial-based ones as shown in \textit{Equation (Equation 8.6)} with the only difference that the basis vector includes a complete set of trigonometric terms instead on monomial terms.

$$\Psi_I(x) = H^T(0)M^{-1}(x)H(x - x_I)\phi_a(x - x_I)$$ \hspace{1cm} (8.24)

This is obvious from the procedure shown above that for reproducing and approximating harmonic (semi-harmonic) functions, both sin and cos terms of the same argument are needed. Otherwise the reproducing conditions could not be satisfied. Considering the same approach for two-dimensional case, in general form, all sin and cos terms of arguments $\omega_x$ and $\omega_y$ must be included in the basis vector. These terms can be shown that are needed for satisfying the reproducing conditions for interactive terms of sin and cos. The first order harmonic reproducing conditions for two-dimensional case can be shown as,
\[ \sum_{I=1}^{NP} \Psi_I(x) = 1 \]  
(8.25a)

\[ \sum_{I=1}^{NP} \Psi_I(x) \sin[\omega_y(x - x_I)] = 0 \]  
(8.25b)

\[ \sum_{I=1}^{NP} \Psi_I(x) \cos[\omega_y(x - x_I)] = 1 \]  
(8.25c)

\[ \sum_{I=1}^{NP} \Psi_I(x) \sin[\omega_y(y - y_I)] = 0 \]  
(8.25d)

\[ \sum_{I=1}^{NP} \Psi_I(x) \cos[\omega_y(y - y_I)] = 1 \]  
(8.25e)

\[ \sum_{I=1}^{NP} \Psi_I(x) \sin[\omega_y(x - x_I)] \sin[\omega_y(y - y_I)] = 0 \]  
(8.25f)

\[ \sum_{I=1}^{NP} \Psi_I(x) \sin[\omega_y(x - x_I)] \cos[\omega_y(y - y_I)] = 0 \]  
(8.25g)

\[ \sum_{I=1}^{NP} \Psi_I(x) \cos[\omega_y(x - x_I)] \sin[\omega_y(y - y_I)] = 0 \]  
(8.25h)

\[ \sum_{I=1}^{NP} \Psi_I(x) \cos[\omega_y(x - x_I)] \cos[\omega_y(y - y_I)] = 1 \]  
(8.25i)

### 8.2.3 System of equations using harmonic-enriched RK shape-functions

Considering the wave equation as,

\[ \ddot{u} = c_0^2 \Delta u \]  
(8.26)
Where \( c_0 \) represents the one-dimensional elastic wave speed defined as \( c_0 = \sqrt{\frac{E}{\rho}} \), the variational form of the wave equation could be derived as,

\[
\int_{\Omega} \delta u \cdot \rho \ddot{u} d\Omega + \int_{\Omega} E \nabla \delta u \cdot \nabla u d\Omega - \int_{\Gamma_d} E \delta u (\nabla u \cdot \mathbf{n}) d\Gamma = \int_{\Gamma_h} E \delta u g_n d\Gamma \tag{8.27}
\]

In Equation 8.27, \( \Omega \) represents the problem’s domain, \( \Gamma_d \) and \( \Gamma_h \) indicates the Dirichlet and Neumann boundaries, respectively such that \( \Gamma_d \cup \Gamma_h = \Gamma \) and \( \Gamma \) is the domain’s boundary. \( \mathbf{n} \) is the outward normal of the boundary and \( g_n = \nabla u \cdot \mathbf{n} \) is the boundary traction.

In mesh-free methods, because of lack of Kronecker-delta property, applying the Dirichlet boundary condition need special treatment. For this purpose, Nitsche’s method is employed for imposing the essential boundary conditions as discussed in Chapter 7. By having the weak-form of the wave propagation problem in hand, the discretized dynamic equation could be written as,

\[
\mathbf{M} \ddot{\mathbf{d}} + \mathbf{K} \mathbf{d} = \mathbf{F} \tag{8.28}
\]

where mass matrix \( \mathbf{M} \), stiffness matrix \( \mathbf{K} \), and force vector \( \mathbf{F} \) in Equation 8.28 are defined as

\[
M_{IJ} = \int_{\Omega} \Psi_I \rho \Psi_J d\Omega \tag{8.29a}
\]

\[
K_{IJ} = \int_{\Omega} \Psi_I E \Psi_J d\Omega - \int_{\Gamma_d} E [\Psi_I \Psi_J, n_i + \Psi_J \Psi_I, n_i - \beta \Psi_I \Psi_J] d\Gamma \tag{8.29b}
\]

\[
F_I = \int_{\Gamma_h} E \Psi_I g_n - \int_{\Gamma_d} E [u_d \Psi_I, n_i - \beta u_d \Psi_I] d\Gamma \tag{8.29c}
\]
8.3 Dispersion and stability properties of harmonic-enriched RKPM semi-discretizations

In order to assess the numerical performance of the Harmonic-Enriched RKPM, the von Neumann method is introduced to investigate the dispersion and stability characteristics. The von Neumann results of Harmonic-Enriched RKPM is carried out for the dispersion of one-dimensional second order wave propagation problem and then compared with the standard RKPM and FEM. In section 8.3.2 the von Neumann is employed to study temporal stability for solving the one dimensional second order wave equation and again the result is compared with standard RKPM and FEM.

8.3.1 Dispersion

For a non-dispersive physical model of wave propagation, the numerical solution of hyperbolic partial differential equations are dispersive due to the discretization. The difference between the numerical wave speed and the exact wave speed can characterize the dispersion errors. In a dispersive medium, the wave speed is a function of frequency or wavelength of the propagating wave. In order to assess the numerical dispersion error of the Harmonic-Enriched RKPM semi-discretization equation, the von Neumann method is utilized. consider the Equation 7.1. The body force is ignored due to concentration on the dispersion associated with the disturbance propagation as a result of initial conditions. The associated spatial semi-discretization of the second order wave equation is as presented in Equation 7.7.

Advancing towards the Fourier analysis, the plane wave of continuum wave can be expressed as:

\[ u(x, y, t) = u_0 \exp[ik_0(x \cos \theta + y \sin \theta) - i \omega_0 t] \]

(8.30)
where $u_0$ is the amplitude, $\theta$ is the propagation direction of the plane wave and for a non-dispersive medium with the wave number $k_0$ and the circular frequency as $\omega_0$ the following relationship with the wave velocity exists:

$$c_0 = \frac{\omega_0}{k_0}$$

(8.31)

The numerical plane wave solution at point $(i, j)$ with coordinates $(x_i, y_j)$ is as follows:

$$u^h(x_i, y_j, t) = u_0 exp[i(k x_i \cos \theta + y_j \sin \theta) - i \omega t]$$

(8.32)

where $\omega$ is numerical circular frequency and $c = \frac{\omega}{k}$ is the numerical wave speed. By considering a uniform spatial discretization $x_{i+m} = x_i + m \Delta x, m + i = 1, ..., NP_x, y_{j+n} = y_j + n \Delta y, j + n = 1, ..., NP_y$, where $NP_x$ and $NP_y$ are the number of points in x and y directions, respectively, the plane wave solution to the semi-discrete equations at point $(i + m, j + n)$ is:

$$u^h(x_{i+m}, y_{j+n}, t) = u_{i,j} exp[i(k (m \Delta x \cos \theta + n \Delta y \sin \theta) - i \omega t)]$$

(8.33)

Let $U(t) = Nd(t)$ be the displacement vector evaluated at points $(x_i, y_j)$. Equation 7.7 can be rewritten in terms of $U(t)$ as:

$$\sum_{i} \sum_{j} \left[ M^*(i,j)(i+m,j+n) \dddot{u}_{i+m,j+n} + K^*(i,j)(i+m,j+n) u_{i+m,j+n} \right] = 0$$

(8.34)

Therefore, the semi-discrete wave Equation 8.34 at point $(x_i, y_j)$ can be expressed as:

$$\sum_{i+m=1}^{NP_x} \sum_{j+n=1}^{NP_y} \left[ M^*(i,j)(i+m,j+n) \dddot{u}_{i+m,j+n} + K^*(i,j)(i+m,j+n) u_{i+m,j+n} \right] = 0$$

(8.35)
Substituting Equation 8.33 into Equation 8.35, we obtain the equation for the circular frequency $\omega$:

$$-\omega^2 \sum_{i+m=1}^{NP_x} \sum_{j+n=1}^{NP_y} M^*_{(i,j)(i+m,j+n)} \exp[ik(m\Delta x \cos \theta + n\Delta y \sin \theta)]$$

$$\sum_{i+m=1}^{NP_x} \sum_{j+n=1}^{NP_y} K^*_{(i,j)(i+m,j+n)} \exp[ik(m\Delta x \cos \theta + n\Delta y \sin \theta)] = 0$$

(8.36)

Introducing the normalized phase velocity $\frac{c - c_0}{c_0}$, where $c = \frac{\omega}{k}$ is numerical phase velocity, we have:

$$\frac{c - c_0}{c_0} = 1 \frac{\sqrt{\sum_{i+m=1}^{NP_x} \sum_{j+n=1}^{NP_y} K^*_{(i,j)(i+m,j+n)} \exp[ik(m\Delta x \cos \theta + n\Delta y \sin \theta)]}}{\sqrt{\sum_{i+m=1}^{NP_x} \sum_{j+n=1}^{NP_y} M^*_{(i,j)(i+m,j+n)} \exp[ik(m\Delta x \cos \theta + n\Delta y \sin \theta)]}} - 1$$

(8.37)

For one-dimension with symmetry, the normalized phase velocity in Equation 8.37 reduces to:

$$\frac{c - c_0}{c_0} = 1 \frac{\sqrt{\sum_{i+m=1}^{NP} K^*_{i,i+m \cos(km\Delta x)}}}{\sqrt{\sum_{i+m=1}^{NP} M^*_{i,i+m \cos(km\Delta x)}}} - 1$$

(8.38)

In the following analysis, a one-dimensional wave equation is considered:

$$\frac{\partial^2 u}{\partial t^2} = c_0^2 \frac{\partial^2 u}{\partial x^2}$$

(8.39)

$M$ and $K$ matrices are constructed by FE, standard RKPM and Harmonic-Enriched RKPM, the domain $0 \leq x \leq L$ is discretized by a set of uniformly distributed points, and wave speed is set to be $c_0 = 1$.

It is worth noting that $M$ matrix is a consistent mass matrix. In order to minimize the boundary effects we consider a relatively large domain with $L = 100$. The number of points are $NP = 101$, with a nodal distance $h = 1$. A non-dimensional wave number defined as $\frac{h}{\sqrt{2}}$ versus normalized phase velocity.
As shown in Figure 42, the dispersion errors are less than 4% for the standard RKPM for any wave length. For the Harmonic-Enriched RKPM case, the error reduces further to 2% when it gets close to the discretization limit \( \left( \frac{h}{\lambda/2} \right) \). As can be seen, Harmonic-Enriched RKPM exhibits much smaller dispersion errors compared to finite elements.

![Figure 42. Normalized wave velocity of FE, standard RKPM and Harmonic-Enriched RKPM](image)

**8.3.2 Stability of harmonic-enriched RKPM with central difference temporal discretization**

The von Neumann method determines the stability by examining the amplification of the Fourier representation of the temporal discretization errors. In the stability analysis, we consider the RKPM
spatial discretization of one-dimensional wave. Considering the central difference temporal discretiza-
tion of Equation 8.26 we have:

\[(U_{n+1} - 2U_n + U_{n-1}) = c_0^2 \Delta t^2 \mathbf{Nd}_n\]  \hspace{1cm} (8.40)

To estimate the stability condition of the full discrete equation in Equation 8.40, we consider the von
Neumann method. Let \(u_m^n\) be the \(m\)th component of \(U_n\), and express it in the following form:

\[u_m^n = \gamma^n e^{imkh}\]  \hspace{1cm} (8.41)

where \(\gamma\) is the amplitude, \(h\) is the nodal distance, and \(k\) is the wave number. By substituting Equation 8.41 into Equation 8.40 and evaluating the \(m\)th row, we have:

\[\hat{m}(\gamma - 1)^2 + \Delta t^2k\gamma = 0\]  \hspace{1cm} (8.42)

By requiring the following condition for bounded solution, we have the stability curve in Figure 43:

\[|\gamma| \leq 1\]  \hspace{1cm} (8.43)

The results show that RK formulations allow a larger critical time step than FEM, which is particularly
noticeable when \(\frac{h}{\lambda/2}\) is closer to 1.
8.4 Numerical examples

A number of problems were analyzed using the RKPM implementation. These include continuous bi-harmonic and 10-cycle sin wave propagations in a bar and the solution of a scalar two-dimensional wave. Details and results of each analysis are given in the sections that follow.

8.4.1 Bi harmonic wave propagation in a bar

In this section we illustrate the performance of H-RKPM by solving a one dimensional wave propagation problem in which the double frequency wave is present as well as the main frequency wave. This type of problem occurs in the solution of nonlinear ultrasonic waves, when the wave with the main frequency is distorted and generates the higher harmonics. To be able to correctly predict the higher harmonics is significant because of their correlation to damage prediction in the material. To simulate
the biharmonic wave phenomena, a bar with length of 5 meters, Young modulus of $3 \times 10^8 Gpa$ and density of $800 \frac{kg}{m^3}$ is considered. The solution of $u$ is governed by:

$$\frac{\partial^2 u}{\partial t^2} = c_0^2 \frac{\partial^2 u}{\partial x^2}$$

(8.44)

in which $c_0 = 1$. The boundary conditions are as below:

$$u(0, t) = 0$$

(8.45)

$$u(L, t) = u_0 \omega_2 \sin(\omega_1 t) + u_1 2 \omega_2 \sin(2\omega_1 t)$$

(8.46)

where $\omega_2 = \frac{8\pi}{L}$ and $\omega_1 = \sqrt{\frac{E}{\rho}} \omega_2$ and $u_0$ and $u_1$ are the amplitude corresponding to the harmonic terms and equal to 1.

The initial conditions for this problem is shown below:

$$u(x, 0) = 0$$

(8.47)

$$\dot{u}(x, 0) = u_0 \omega_1 \sin(\omega_2 x) + u_1 2 \omega_1 \sin(2\omega_2 x)$$

(8.48)

And the analytical solution of the wave is as follows:

$$u = u_0 \sin(\omega_2 x) \sin(\omega_1 t) + u_1 \sin(2\omega_2 x) \sin(2\omega_1 t)$$

(8.49)
This problem was analyzed using H-RKPM, RKPM, enriched FE and FE method. For H-RKPM, basis described in section 8.2.3 is utilized with analytical solution’s main frequency in the harmonic terms. A B-spline formulation is used for the kernel. 11 points are used for the discretization. Newmark trapezoidal rule with a time step size of $1 \times 10^{-5}$ s is used for dynamic analysis. For the standard RKPM, Linear basis functions were employed and a B-spline was used for the kernel. At least 100 elements must be used to get acceptable results and a $5 \times 10^{-6}$ s is employed for the time step size. Enriched FE is used with 20 elements, 105 degrees of freedom are generated as a result of using harmonic functions and their double frequencies and same time step size as H-RKPM. Standard FE is used with 200 elements and $5 \times 10^{-6}$ s time step size. The wave profiles of the problem solved with above-mentioned methods and the absolute error ($e_h = u_{exact} - u_{numerical}$) are presented below:

Figure 44. a) Wave profile of bi-harmonic wave propagation in a one-dimensional bar  b) Error comparison
As can be observed in Figure 44, H-RKPM approximates the solution with considerably fewer number of points compared to other methods. Time history of the biharmonic wave problem and the associated error are as given in Figure 45.

![Figure 45. a) Time history of bi-harmonic wave propagation in a one-dimensional bar b) Error comparison](image)

Figure 45. a) Time history of bi-harmonic wave propagation in a one-dimensional bar b) Error comparison

Figure 45 it is observed that H-RKPM performs very well. The frequency responses presented in Figure 46, the newly proposed method has approximated both the fundamental wave and the second-harmonic’s frequencies more accurate than other methods with lower computational cost.

8.4.2 10-cycle Sin wave propagation in a bar

Another one dimensional wave propagation problem with sin wave excitation is solved with H-RKPM, RKPM, enriched FE and FE. A Hamming windowed tone-burst consisting of 10 cycles at a fre-
Figure 46. Frequency response

frequency of $32 \times 10^3 \frac{\pi}{T}$ is used as the excitation signal. A tone-burst Hamming window is used frequently when dealing with ultrasound testing problems. Therefore this one dimensional problem provides insight into numerical modeling of high-frequency ultrasound wave as the frequency prediction becomes important when correlating with the nonlinearities in materials. The Hamming window formulation used is shown below:

$$h(t) = A(0.5(1 - \cos(2\pi \frac{f}{N}t)\sin(2\pi ft))$$  \hfill (8.50)

In which $h$ is the amplitude of the windowed tone-burst signal, $A$ is the amplitude of the excitation, $f$ is the excitation frequency and $N$ is the number of cycles used. The solution is governed by Equation 8.44.

H-RKPM and RKPM, enriched FE and FE are discretized using 81 degrees of freedom within the domain, and for the first three method a time step size of $1 \times 10^{-5} s$ is used and for the standard FE
solution a time step size of $5E - 6s$ is used to get acceptable results. Newmark trapezoidal rule is chosen for the implicit dynamic analysis. The results are compared with the analytical solution. The wave profile and frequency responses are shown below: As can be observed in the results, with

![Wave Profile](image1.png)

![Frequency Response](image2.png)

Figure 47. a): Wave profile of hamming one dimensional wave, b) Frequency response

same discretization, RKPM, enriched FE and FE show oscillations in the solution. However, H-RKPM performs very well which can be observed in approximating the frequency response too.
8.4.3 Solution of a scalar two-dimensional wave

The scalar wave equation with a Ricker wavelet source at the center of a two-dimensional domain is modeled. The governing equation of the solution is:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + F(0, 0, t) = \frac{1}{c_0^2} \frac{\partial^2 u}{\partial t^2} \tag{8.51}$$

in which:

$$F(0, 0, t) = 10(1 - 2\pi^2 f^2(t - 0.25)^2)\exp(-\pi^2 f^2(t - 0.25)^2) \tag{8.52}$$

where $u$ is the displacement solution, $c_0$ is the wave velocity (in this example $c_0 = 1$), $f$ is the central frequency, (in this example $f = 6\text{Hz}$). Due to symmetry, only a quarter of the area is used for numerical solutions which is a $[0, 1] \times [0, 1]$ domain. Generally, in dealing with wave propagation problems, absorbing boundary condition is used, however, here for the time considered 0.95s, the wave does not get to the boundary, hence there will be no reflections and no need for the absorbing boundary conditions. H-RKPM, RKPM, enriched FE and FE models have been discretized with 40 by 40 mesh. The 200 by 200 discretization solution is used as a reference. In all models, Newmark trapezoidal rule of time integration with time step size 0.00625s is used.\textcolor{red}{8.4.3} shows snapshots of the wave at 0.95s for all the simulations. Wave profiles and frequency responses are presented and compared at \textcolor{red}{8.4.3}

For the given discretization, FE and enriched FE give results not as good as obtained with H-RKPM and RKPM. H-RKPM approximation matches well with the analytical solutions, providing us with a more accurate and efficient solution for the scalar two-dimensional wave problem.
8.5 Discussions and conclusion

A Harmonic-enriched Reproducing Kernel Particle Method for solving high frequency wave propagation problems in solids with higher accuracy has been presented. Following the same procedure for constructing polynomial-based RK shape functions, a set of harmonic terms are introduced into the basis vector to satisfy the harmonic reproducing conditions and therefore accurately approximate harmonic and semi-harmonic functions. The constitutive models originally developed for FEM models can be implemented as Harmonic-enriched RKPM is developed based on the Galerkin formulation.

Since the H-RKPM approximation is constructed based on Fourier terms, the method is capable of handling various range of wave propagation problems with more accuracy and less computational cost than the traditional methods. In particular, tuning the frequency of the harmonic terms used in the basis vector can provide a means to improve the results even further.

The dispersion and stability properties shown to be better than the traditional methods, ensuring the higher numerical accuracy in wave propagation problems.

The solutions are compared with the traditional RKPM and FE. In addition, same harmonic terms are added to the nodes of standard FE elements as additional degrees of freedom, making an explicitly enriched FE and the results are compared. The use of the method is illustrated in one-dimensional and two-dimensional solutions, but the concept directly applies to three-dimensional solutions as well. Both H-RKPM and enriched FE require special attention while imposing the boundary condition.

The method requires additional harmonic terms in the basis functions as the discretization gets coarser. However, this is done without adding to the degrees of freedom, therefore, the computational
cost is still lower than explicitly enriching the numerical method. In this way, accurate solutions can be obtained with reasonable meshes and solution data.

According to numerical results, H-RKPM performs very well in wave propagation problems and does not show redundant oscillations in the solution which is crucial for frequency response analyses.

In further research on the method, some problems should be tackled. In this paper, the potential of the method to spatially resolve the desired solution is assessed and the computational cost is not analyzed directly. Hence further research should primarily focus on reaching cost effectiveness when using the method. For transient analyses, we have employed the method with a consistent mass matrix and implicit time integration schemes, and obtained accurate solutions. However, the use of lumped mass approximations and explicit time integration, typically used for wave propagation solutions, should be explored. The numerical integration of the stiffness and mass matrices should be studied in detail with the aim to find optimal schemes. We used the standard Gauss integration rules with many integration stations on the elements as the harmonic term numbers increases.

The method has good capability for the analysis of nonlinear ultrasonic problems as it can tackle high frequency wave problems more accurately and with less computational cost. The results showed that H-RKPM is a better predictor of the fundamental and higher-harmonics in the wave propagation problems. However, the solution of nonlinear wave propagation problems can be considered for future studies.
Figure 48. Wave snapshot at 0.95s a) FE b) Enriched FE c) RKPM d) H-RKPM e) Analytical solution
Figure 49. a) Wave profile at 0.95s b) frequency response
CHAPTER 9

CONCLUSION AND FUTURE WORK

9.1 Conclusions

The concluding remarks of thesis are divided into two topics.

In NLUT, the measurement of the amplitude of higher harmonics is required. This measurement is derived from the frequency response of the ultrasonic signal. In order to enhance the measurement of the higher-order-harmonics, the signal processing methods based on the FFT and the WT utilizing an analytical solution as the input signal are compared and the calculated $\beta$ from the WT method is seen to agree well with the analytical solution regardless of the input amplitude while the result from the FFT displays strong dependence on the amplitude. This dependence becomes problematic as an inherent material property should not be dependent on the excitation amplitude or frequency. WT can successfully overcome this issue and as a result a WT-based NLUT is established.

The WT-based algorithms are introduced to obtain the relative second harmonic-based and third harmonic-based acoustic nonlinearity parameter $\beta'$ and $\gamma'$. The wavelet-based schemes are employed to investigate the change of relative acoustic nonlinearity parameters caused by plastic deformation in heterogeneous media. Several heterogenous models are simulated with statistically variable heterogeneity characteristics and the correlation between these characteristics and higher harmonics are assessed. It is shown that the third harmonic is an effective tool to detect damage in heterogenous media. Moreover, the standard deviation of material strength is shown to have the utmost significance compared to
other heterogeneity properties like volume fraction and heterogeneity size in the generation of higher harmonics. In addition to the above, it is shown that explicit modeling of heterogeneities once and only at the beginning of analysis, equips the simulation with sufficient information for undergoing any future types of loading, hence monitoring the change in the model more efficiently.

The material nonlinearity is observable in the ultrasonic signal through the generation of higher-order-harmonics (HOH). The HOH generation, however, can be triggered by many sources. Any variation in the micro-, meso-, and macroscopic scales of the structure may collectively lead to HOH generation. A finite element approach with mesoscale heterogeneities explicitly modeled for the nonlinear wave propagation is presented. The aim of this study is to understand HOH generation due to the non-mesoscale variation and non-uniform deformations introduced by the uniaxial tensile test. This study is divided into two parts: First, the effect of non-uniform plastic deformation resulted by geometrical variation of structures on HOH is studied. Next, the effect of non-uniformity due to mesoscale variations on HOH is analyzed. For this purpose, WT-based algorithms are applied to measure the acoustic nonlinearity parameter. The numerical studies and predictions are crossly validated with nonlinear ultrasonic experiments and microscale imaging, including X-ray Diffraction (XRD) scanning. Numerical and experimental studies both indicate that non-uniform variations in different length scales affect the generation of both the second and the third-harmonics, and that both second- and third-harmonics acoustic nonlinearity parameters grow with the increase of plastic strain level. However, the third-harmonics acoustic nonlinearity parameter is more sensitive when micro-, meso- and macrostructural variations exist. Accordingly, this parameter is a more beneficial indicator of nonlinearity in materials when non-uniform deformation is present.
Since the frequency of ultrasonic signals are generally high, extremely fine mesh is required to obtain reasonable solution particularly in nonlinear wave problems. Therefore, the second part of this thesis is devoted to the development of an enriched numerical model to solve for linear and nonlinear wave propagation problems and handle them more effectively. Two specific enriched methods are developed: enriched FE and Harmonic-Enriched RKPM. In enriched FE, standard FE shape functions are enriched with the characteristic solution of the wave propagation problem which are harmonic functions. The primary advantage of this approach is that all the fundamental properties of standard method is applicable. Moreover, when solving for nonlinear UT problems, the fact that the excitation frequency and higher harmonic frequencies are already known, accents the benefit of applying enrichment functions that can accurately capture the characteristics of the solution. The method is verified by comparing with standard FEM and the analytical solution of the wave propagation in hyperelastic media. Since the enrichment function does not possess Kronecker delta property, the Nitsche’s method is introduced for applying the boundary, which leads to better solution accuracy. In order to solve for large scale nonlinear wave propagation, a User Element is implemented and incorporated into Abaqus. The results from comparing enriched and standard FE shows enriched FE has improved efficiency and accuracy in nonlinear wave propagation problems. Overall, enriched FEM is proved to be an effective method for nonlinear wave propagation problems, hence applicable to effectively predict the ultrasonic waveform and quantify the damage.

In order to even further reduce the computational cost and benefit from the advantages of element free methods, Harmonic-enriched RKPM (H-RKPM) is introduced. The method is developed based on an implicit enrichment formulation under the RKPM framework. The desired harmonic function is
introduced as the basis function for construction of reproducing kernel and the reproducing condition is enforced. This approach allows the characteristic function to be embedded in the approximation without adding more degrees of freedom. As a result, the high frequency wave problem can be solved using fewer nodes, enhancing both computational efficiency and accuracy. The dispersion analysis shows the method is more accurate than the standard RKPM with the same discretization. Stability analyses predicted the critical time step sizes for H-RKPM to be larger than standard RKPM and FE. The performance of this method is demonstrated using one-dimensional and two-dimensional benchmark problems. H-RKPM also requires special attention while imposing the boundary condition. Nitsche’s method is used to apply the essential boundary conditions. The method was capable of predicting the higher harmonics amplitude more accurately when compared with standard RKPM, enriched FE and FE.

9.2 Future work

The future work that can be extended from this thesis should focus on the numerical issues that require further studies and enhancements of the current numerical frameworks for the nonlinear wave propagation modeling. It can be summarized as follows:

1) H-RKPM and enriched FE both need many Gaussian integration points for the domain integration in the Galerkin formulation. Domain integration methods can still be improved to enhance stability and efficiency, while preserving accuracy.

2) In this thesis, consistent mass matrices and implicit dynamic approach is utilized to solve the wave propagation problems. However, lumped mass and explicit dynamic methods are attractive in wave
propagation problems due to their computational efficiency. Implementation of the explicit dynamic method is suggested.

(3) The implementation of H-RKPM in nonlinear wave propagation problems are suggested. In this thesis, the nonlinear wave propagation solver by enriched FE was modeled through a User Element in Abaqus and the results were compared with nonlinear FE. Implementing the same technique to observe H-RKPM’s performance in nonlinear wave propagation can be of interest.

Moreover, the numerical NLUT simulation can be improved and applied to other damage types such as follows:

(4) Different microstructural damage types like creep are suggested to be considered and incorporated using microstructural images and the correlation between these damages and higher-order-harmonics can be investigated numerically.

(5) Multiscale framework is suggested to be established to effectively simulate nonlinear ultrasonics in media with microstructural evolution. The microstructure of material at different scales collectively causes the material nonlinearity and affects the wave propagation properties. However, modeling detailed microstructure of material directly from the dislocation scale to the structural scale is practically impossible. Thus, multiscale modeling can be introduced to provide us with better predicting the received ultrasound and understanding its characteristics.
9.3 Acknowledgement

This Preliminary research is based upon work supported by the National Science Foundation (NSF) under award number CMMI 1463501 entitled ”Assessing Microstructural Damage Using Nonlinear Ultrasonics and Multiscale Numerical Modeling”. Dr. Daniel P. Bailey, University of Illinois at Chicago College of Engineering, contributed to the copy editing of Chapter 6 of this manuscript.


81. Griffiths, J. R.: DAMAGE BY THE CRACKING OF SILICON PARTICLES AN AL-7Si-0.4Mg CASTING ALLOY. 44(1):25–33, 1996.


127. ongpeng: UTILIZATION OF NONLINEAR ULTRASONIC PROPERTIES IN DETERMINING INTERIOR Utilization of Nonlinear Ultrasonic Properties. (May), 2015.


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