DPAI: In-Situ Process Intelligence using Data-Driven Simulation-Assisted-Physics Aware AI (DPAI) for Simulating Wave Dynamics

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Abstract

AI models such as convolutional long short-term memory (ConvLSTM) recurrent neural network (RNN) have been shown here to have the capability to simulate ultrasonic wave propagation in the 2-D domain. This DPAI approach uses the Data-driven but simulation-assisted-Physics aware approach to utilizing **AI** networks. Our DPAI model comprises ConvLSTM with an encoder-decoder structure, which learns a representation of spatio-temporal features from the input sequence datasets. The DPAI model is trained with finite element (FE) time-domain simulation datasets consisting of distributed single and multi-point source excitation in the medium, reflection from the simple boundaries, and phased array steering. Here, this approach, called the DPAI model, is demonstrated for modelling multiple point sources to simulate forward wave propagation, reflection from the boundaries, and phased array beam steering ultrasound wave dynamics in a 2D plane. The trained DPAI model was found to be significantly faster in generating simulations for the time evolution of field values in the elastodynamic problem when compared to the conventional finite element explicit dynamic solvers.

Keywords: *DPAI, Ultrasonic Wave simulation, Phased Array, FE, Deep Learning, RNN, ConvLSTM.*

1 INTRODUCTION

Ultrasonic wave propagation has wide-ranging applications in several fields, such as geological investigations, seismic research, non-destructive evaluation [1], and biomedical imaging. Improving our comprehension of the physics behind these applications depends heavily on the numerical modelling of ultrasonic wave propagation. The transitory nature of wave propagation and the three-dimensional region in which the wave is to be modelled result in enormous processing resources and calculation times, which restricts the use of modelling in real-time field inspection. Numerical models such as Finite Element [1-2], Finite Difference [2], Finite Integrals [3], Galerkin Meshless [4], and other comparable techniques have been employed for modelling wave propagation simulations. The adoption of Graphical Processing Units (GPUs) with parallel computing models for wave propagation [5-6] and several other advancements in mesh discretization and computation have resulted in these techniques that are quicker and need less processing power.

The FE simulation is, nonetheless, widely used for simulating ultrasonic simulations out of all numerical techniques [7]. By solving the wave equation's partial differential equation with specified boundary conditions, the FE simulation offers precise solutions for the most complex problems involved in solving wave dynamics for various geometry and boundary conditions. However, as the number of FE elements/nodes increases, it is generally known to be computationally costly, especially for realistic problems such as higher inspection frequency ranges and larger geometrical domains [8]. Due to its high memory requirements, it is mainly utilized for experimental validation or to create a proof of concept for the ultimate design iteration. An alternate strategy is to create a data-driven solution for wave propagation modeling by extracting the physics from numerical simulation datasets [9-10].

Larger training datasets becoming available, algorithm advancements, and exponential increases in processing power have all contributed to an unprecedented rise in interest in deep learning algorithms in recent years. Massive amounts of input data, particularly high-dimensional datasets [12], could be effectively classified [13], regressed [14-15], clustered [16], or have their dimensionality reduced using deep learning algorithms. Therefore, one of these deep learning models could be used to generate wave propagation, depending on the structure of the datasets being available [17-19]. Since these training datasets include both temporal and spatial characteristics, recurrent neural network (RNN)-based techniques are thought to be the best for simulating the propagation of ultrasonic waves [20-21]. Contemporary deep learning systems like long short-term memory (LSTM), a specific kind of RNN structure employed for diverse applications in science and engineering, can handle vanishing gradients and create long-range temporal representations due to their inherent capacity [22-23]. Convolutional LSTM (ConvLSTM) might be utilized instead of this algorithm as it is less successful at extracting spatial information from the training dataset. In order to complement the temporal state with spatial information, the convolutional operation is used inside the LSTM cell [24-27].

In this work, we present a novel methodology for developing a hybrid Data-driven-Physics-based AI (DPAI) model for simulating ultrasonic wave propagation in real-time. This involves a supervised learning model obtained from deep convolutional long short-term memory (ConvLSTM) networks [28-30]. Our earlier research demonstrates the modeling of wave reflection from boundaries with varying physical settings and forward wave propagation simulation [31]. Additionally, in order to simulate phased array beam steering wave simulation in a 2D domain, the authors wish to expand the DPAI model widely. This study presents the development of three distinct DPAI models. The training datasets for the first DPAI model are created by simulating the time domain FE simulation of multiple point excitation sources inside the solid medium of forward wave propagations. This model is then utilized to model different multiple-point source excitation simulations. Similar to the first DPAI model, the second one is trained using a collection of FE ultrasound wave simulations, which provide the training data for single-point excitation at the medium's top surface with different 2D geometrical shapes. The phased array (PA) ultrasound technique is the most extended for defect detection and characterization in the NDE domain because of the ability to focus and steer the beam without the physical movement of the transducer. The primary advantage of the PA technique over the conventional ultrasonic technique is that large regions can be inspected from a single location using various ultrasonic profiles such as plane wave and beam steering and focusing without disturbing the transducer position, which is a much faster process. Therefore, we have modeled the 16 active elements phased array probe with variable angles of -40 to 70 degrees in FE to produce the training dataset for the third DPAI model. In order to extract the temporal evolution and spatial feature information of ultrasonic wave mechanics, the DPAI network design uses a convolutional LSTM encoder-decoder structure.

Using this DPAI model, it is shown to be feasible to model simulation with significantly reduced time and resources for computation that compares well with the FE model outputs. Furthermore, the DPAI, like most data-driven models, is based on algebraic calculations, and the computational resource requirements are significantly reduced compared to conventional numerical approaches.

This paper is organized as follows: Section 2 describes the DPAI training datasets created using Finite Element Analysis. The formulation of the wave propagation problem using the DPAI algorithms is detailed in Section 3. Numerical experimentation and results are given in Section 4, and Section 5 concludes the work.

2 SIMULATION-ASSISTED TRAINING DATA SET GENERATION FOR DPAI:

The AI model learns the principles of ultrasonic wave propagation while it trains the network to produce real-time simulations. This work uses the FE simulation method to obtain the bulk datasets needed for training the DPAI. This section provides a detailed description of the generation of the simulation-assisted data collection.

2.1 Finite Element Modelling for Transient Wave Dynamics in the 2D domain:

Large amounts of simulated-assisted data are required for the AI-enabled wave propagation in solids, and these are created by modelling FE simulation in the time domain. Abaqus/Explicit

Dynamics Solver, an FE software package, is used to solve the physics-based wave equation. A comparable 2D plane strain CAD model is created using a 35 x 35 x 20 mm test sample of carbon steel. The bilinear quadrilateral element is used to discretize the 2D domain into 22 elements per wavelength (longitudinal wave velocity). The FE nodes function as transmitter-receiver pairs by establishing a standard ultrasonic transducer location. To avoid the undesired reflections from ends, ALID (absorbing layers using increasing damping) applies the absorbing boundary conditions on all sides of the plate [32]. The two-cycle Hanning windowed tone burst signal of 5 MHz inspection frequency is used to excite the ultrasonic pulse of an incident wave given in function of time. The pulse excitation is applied in terms of single/multiple concentrated forces on nodes that act as the physical transducer. Figure 2(a) reports the three excitation point sources in the FE model. The sequence of the displacement plot over the total simulation time is extracted for every successful completion of the analysis. A similar approach is followed from our prior work for modeling [27].

In this work, we aim to teach DPAI the physics of wave propagation by creating different 2D CAD models based on the probability distribution function (PDF) by computing critical transducer position parameters to generate a bulk quantity of training simulation data sets. The critical transducer position parameters are calculated using PDF based on the influence of real-time experimentation, such as expected loading direction, position probabilities, number of excitations point sources, the sensitivity of instruments, etc. We have generated three different datasets to develop three different DPAI models. In the first type of dataset, a one-direction load is applied per simulation in terms of concentrated force either in the X or Y-direction in the FE modelling, which is randomly located in the test sample area. The excitation point source is distributed from single to five excitation point sources. A total of 500 FE simulation sequences of the frame dataset are created.

In the second type of dataset generation, we modelled three distinct geometrical CAD models with physical dimensions of 40 x 40 mm overall. Excitation load is applied to the top-edge nodes of 1000 CAD models, each with three distinct form domains, as shown in *Figure 5(a)-(c)*. These models are then solved in FE simulation. All other CAD model surfaces have traction-free boundary conditions applied to them in order to permit reflections off the side and rear walls.

The third generation of datasets involves solving the governing wave equations in FE using initial and boundary conditions of the phased array of active elements. Using a predetermined focal law that has been computed for beam steering, the 16-element active aperture in the PAUT approach is activated. These delay laws are fed into the Abaqus to model the concentrated force as the emitting source in the medium. All the active aperture elements are triggered in parallel using pre-defined delay laws to form the ultrasound beamforming to steer in the medium, and the FE simulation snapshot is shown in *Figure 7(a)***.** A total of 600 FE simulations is created by applying the delay laws of each beam steering angle. The steering angle used for simulation lies between -40 degrees to 70 degrees.

Generating one FE simulation takes 40 minutes using time-domain FE analysis executed using a Dual Intel Xeon Platinum 8168 processor with 48 cores and 1000 GB RAM. Hence, this conventional explicit dynamics FE analysis is time-consuming for design iteration. We have introduced the DPAI network to generate synthetic wave dynamic simulations to overcome this.

3 MODELLING WAVE PROPAGATION SIMULATION USING DPAI

In the Deep Machine Learning framework domain, recurrent neural networks have played a vital role in modeling spatio-temporal sequence output. The DPAI model architecture used for modeling wave propagation simulation is discussed in detail in the following section.

The LSTM is a unique RNN structure modeled for addressing vanishing gradients and learning long-range dependencies. The LSTM shown in *Figure 1(b)* consists of the following elements: a memory cell C_t, which can accumulate and forget the state being tackled from time-step to time-step. The input gate i_t controls the weather to include new information in the memory cell. The forget gate f_t is responsible for removing information from the cell state, and an output gate O_t is responsible for transferring information from C_t to hidden state H_t. The hidden states could retain the memory of past knowledge and learn the long-range dependencies in sequence data. The LSTM network is successful in many domains, but it will be a poor choice for modeling wave propagation problems, which is overcome by implementing a convolutional LSTM network. In this network, the higher dimension matrix multiplications are replaced with the convolutional operation, which reduces the number of training parameters and maintains the spatial features intact [24]. The key equations for the ConvLSTM network are as follows from our prior work [28].

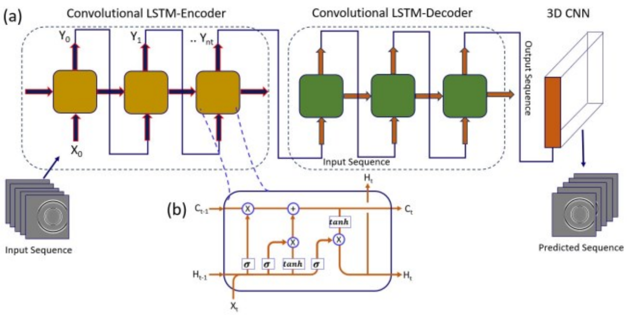


Figure 1: ***(a)*** *Typically DPAI stacked convolutional LSTM encoder-decoder architecture for modelling wave propagation phenomenon. (b) Structure of a single convolutional LSTM cell.*

The DPAI network algorithm is a combination of a convolutional neural network (CNN) and a recurrent neural network (RNN). We have used the proposed DPAI network for our spatial-temporal sequence generation problem, as shown in *Figure 1(a)*, consisting of an encoder and a decoder network containing two convolutional LSTM cells stacked together. Each input sequence is fed into a new encoder ConvLSTM cell together with the hidden state from the previous ConvLSTM cell. The encoder processes input iteratively through various ConvLSTM cells and outputs embedding tensor, representing wave propagation. The output of the encoder-embedded tensor is fed to the decoder network to produce a predicted wave propagation simulation. The decoder cell outputs the sequence of feature maps for each predicted frame. These feature maps are transformed into actual predictions using 3D CNN layers with a sigmoid activation function.

4 NUMERICAL EXPERIMENTATION AND RESULTS USING THE DPAI MODEL

In the following section, ultrasonic wave propagation physics is taught to the DPAI model while training the network to generate the synthetic elastodynamic simulations is discussed in detail. The DPAI architecture is implemented based on the dataset generated in section 2. The qualitative and quantitative results of trained three different DPAI model performances on wave propagation datasets are described in detail in this section.

4.1 DPAI model training and testing on forward wave propagation simulation:

To train the artificial intelligence algorithms needs a large number of training data sets for better performance. The proposed DPAI model is trained using FE-generated simulation-assisted training sequences created using a single excitation to multiple point excitation sources applied as triggering signal pulse. These training data sets are extracted from FE simulation as the sequence of images over 5 microseconds with a sampling time interval of 0.74 microseconds per frame. These simulation data are extracted as frames over 5 microseconds with an interval of 0.74 microseconds per frame. We have created a total of 1000 simulation data sets from FE analysis. These sequences contain 675 frames per simulation. Each simulation is divided into a mini-batch of 12, and each mini-batch contains 15 sequences of frames. The total mini-batch is split as 80% for training, and the remaining 20% is used for testing. Each sequence of frames is further divided into 10 for the input and 5 for the ground truth. Although the input sequence and ground truth instances are sliced from the same simulation having dependencies, this splitting strategy is still reasonable because, in real experimentation, we have access to the previous and successive subsequent frames, which allows us to predict the full-length simulations. These datasets are in greyscale with pixel values of range [0, 255], normalized from [0,1] pixel values with a size 256 x 256.

The proposed DPAI model is implemented in PyTorch-lightning [33-34], an open-source framework that is great for removing many boilerplate codes and integrating multi-GPU training. The DPAI architecture shown in Fig. 2 consists of four layers of encoder-decoder structures stacked together. Each layer contains 256 hidden states with a 5 x 5 kernel size. A mini-batch size of 12 sequences is drawn from a random distribution as input to the network. The DPAI network is trained to minimize the Mean Square Error (MSE) loss function using the back-propagation through time (BPTT) algorithm. The network's learnable hyperparameters are initialized to zeros to prevent the instability of the network. The Adam optimizer is used to optimize different network weights and biases with a learning rate set to 0.0001 and trained for 200 epochs.

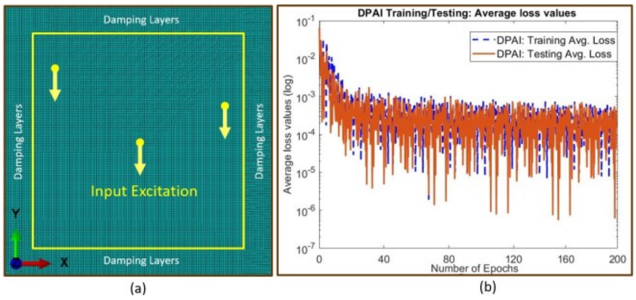
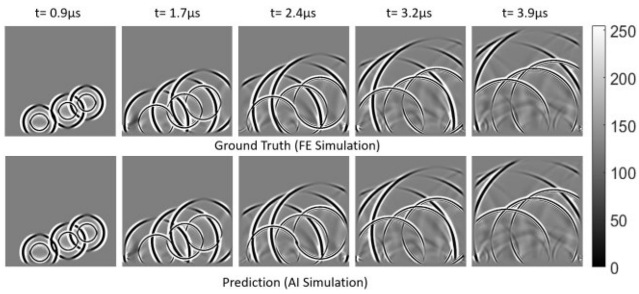


Figure 2: (a) *An example of the FE model, where the incident wave is triggered by modelling the three excitation point sources. The absorbing boundary condition is applied to all wall sides with different damping coefficients to prevent undesirable effects.* ***(b)*** *DPAI: Training/Testing: the forward wave propagation dataset's average loss values over the number of epochs.*

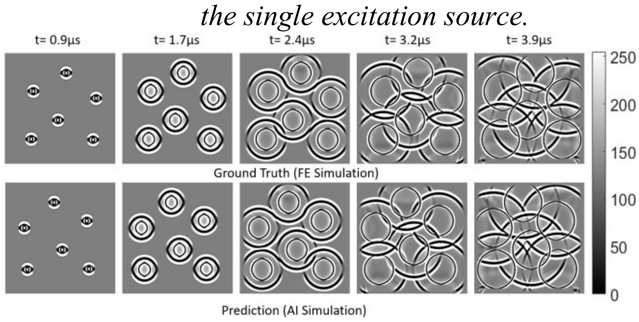
The average loss metric is used to measure the performance of the network while training. The loss is calculated by comparing the network-predicted simulation with ground truth simulations. *Figure 2* shows the average loss values over the number of iterations. The average loss values are stabilized over the iterations; thus, the network's predicted sequence of images is comparable with the ground truth sequence of images. The training loss for the entire data is 0.00038 for 260k iteration, and the testing loss is 0.00052. Training and testing execution is done on NVIDIA GeForce RTX 3090 dual GPU machine. The time taken to train the DPAI model is about 32 hours.

We have used a trained network as a predictive model for emulating time-domain ultrasonic wave propagation. We have adopted a continuous prediction strategy for predicting the successive 5-frames in a sequence by continuously providing the previous 10-frames as input to the DPAI model. We have provided an initial input mini-batch of frames from FE analysis; then, the predicted frames are given as input to form a closed loop for predicting the entire simulation. This procedure continually loops until all frames are anticipated until total frames are generated in a simulation. In this procedure, frames from the FE simulation are supplied for the first iteration, and the result from the previous iteration is used as input to forecast the next set of frames for the succeeding iterations.

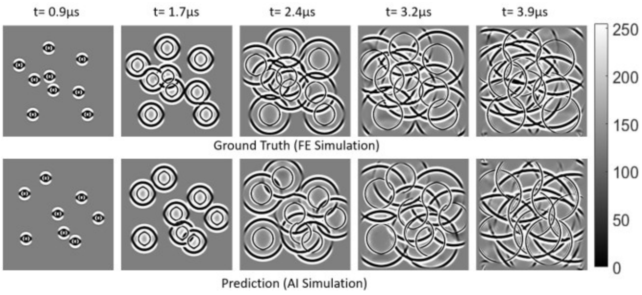
We have modeled three different FE simulations with three excitation, six excitation, and nine excitation point sources to predict the forward wave propagation simulation. To determine the trained network's efficiency, we need to examine qualitatively by comparing the DPAI-modeled simulation with the FE simulation and comparing the A-scan extracted from the AI-predicted simulation and FE simulation at model center pixel locations within the frame. Training and testing execution is done using the same computer hardware. The predictive network takes approximately 2 minutes to generate 675 frames of a single simulation. With this approach, we could successfully reduce the computational overhead to a greater extent, which is 20X faster than the conventional FE solver.



(a) *Comparison between AI/FE simulation for the single excitation source.*

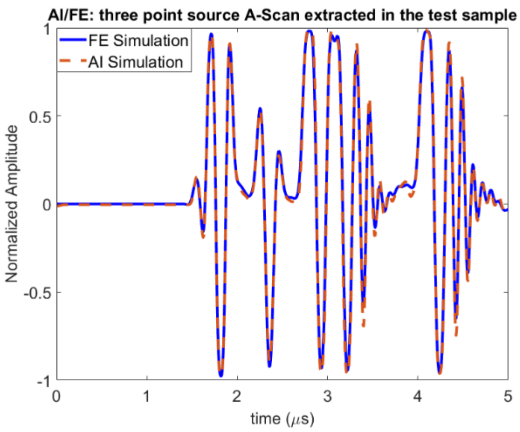


(b) *Comparison between AI/FE simulation for four excitation sources*

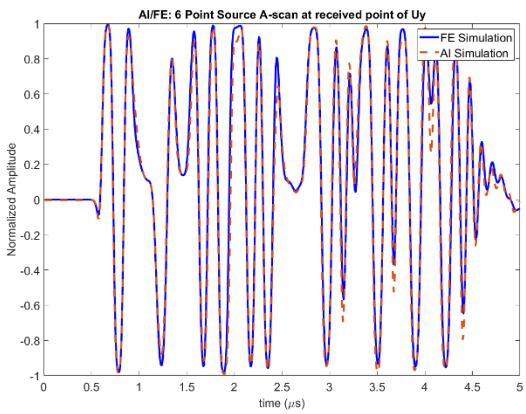


(c) Comparison between AI/FE simulation for five excitation sources

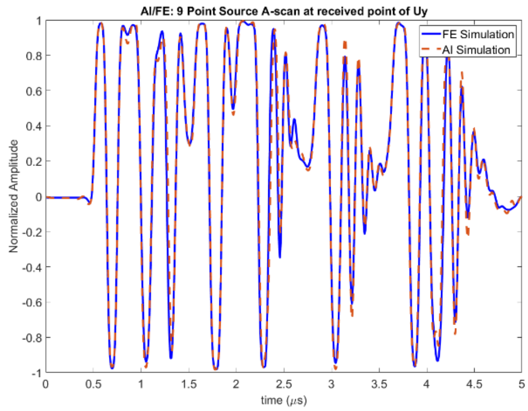
Figure 3*: A qualitative comparison between FE simulation with DPAI-generated simulations for the deeper time period of* ***(a)*** *three,* ***(b)*** *six, and* ***(c)*** *nine excitation sources for spatial features information and time evolution of ultrasonic wave dynamics.*



(a) Three excitation point sources: A-Scan



(b) Six excitation point sources: A-Scan



(c) Nine excitation point sources: A-Scan

Figure 4*: Extracted FE simulation-based A-Scan is compared with DPAI predicted simulation-based A-Scan to validate the effectiveness of the DPAI predictive model for wave propagation simulations at the centre of the frame's location for three* ***(a)****, six* ***(b),*** *and nine* ***(c)*** *excitation sources.*

Figure 3(a)-(c) shows the wave propagation phenomenon evaluation over time for three, six, and nine excitation sources. *Figure 3(a)* describes the three excitation sources for spatial feature evaluation of FE and DPAI simulations over time. *Figure 3(b)* shows the ultrasonic wave propagation evaluation for six excitation sources for the top row FE and the bottom AI predicted simulation. Finally, *Figure 3(c)* evaluated spatial-temporal wave dynamics in the solid medium for nine excitation sources on top-ground truth and bottom DPAI. As seen in *Figure 3*, the predicted frames are identical to the ground truth; these are qualitatively in good agreement in terms of constructive-destructive interference at wave interaction and spatial feature evaluation. We have extracted an A-Scan at a center location inside DPAI-predicted and FE simulation frames to validate each predicted frame, acting as the transducer position shown in

Figure 4(a)-(c) for three, six, and nine excitation sources, respectively. The A-Scan is used to identify the error between the predicted and ground truth for each frame at the transducer location. We have observed that its magnitude falls within 2% error for all the scenarios A-scan according to mean square error over the entire simulation; it will be true as long as the field values are not entirely zero.

4.2 Simulating Reflection Wave Propagation from Irregular Boundaries Using the DPAI Model:

The second DPAI model is trained using the dataset obtained for reflection borders to model the propagation of reflection waves at irregular edges. A similar training methodology is employed to train the DPAI, described in section 4.1. With the exception of the number of epochs and the kernel size being altered to 3 x 3, the DPAI model architecture and layer count are comparable to section 4.1. There are 256 hidden dimensions in every encoder or decoder structure. Over 400 epochs, the average loss value is 0.00042, and the testing loss value is about 0.00068. *Figure 5(b)* shows that the loss value stabilizes as the number of epochs grows. 45 hours are needed to train the DPAI model using an NVIDIA GeForce RTX 3090 dual GPU machine.

In order to expand the scope of the DPAI model, we have examined the propagation of ultrasonic waves in two distinct irregular geometrical domains. A comparison is made between the FE and the anticipated simulation of the DPAI model. *Figure 6* shows the reflected ultrasonic wave propagation for irregular geometrical shapes. *Figure 6* has simulations from the FE in the top row and the

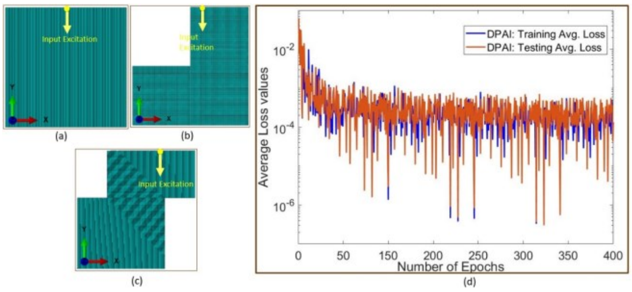
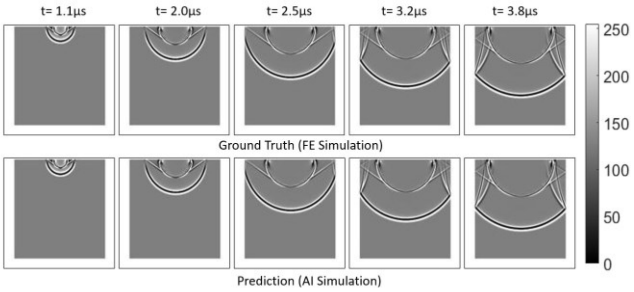
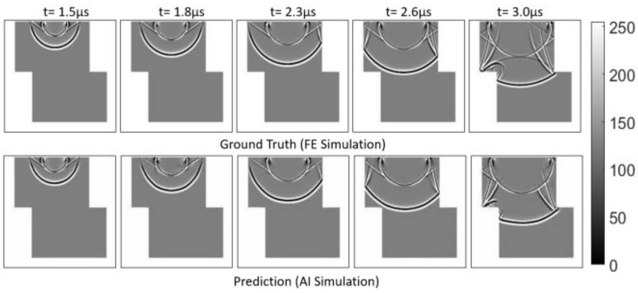


***Figure 5**: **(a)** Finite element models: To create the training dataset, FE models with single point sources are excited in the Y direction at the top surface of the domains. **(b)** DPAI: Training/Testing: The model was trained using the reflection from the boundary datasets, the model average training, and the testing loss throughout the number of epochs.*



***(a)** FE/DPAI simulation comparison for the rectangular boundary.*



***(b)** FE/DPAI simulation comparison for the irregular geometry*

***Figure 6**: Reflected wave propagation with irregular geometrical boundaries: The DPAI model is implemented to simulate the wave propagation simulation in the various irregular geometrical domains. The sequence of frames generated using FE and DPAI simulations are compared at multiple time instants. The 5 MHz central frequency with two cycles is used to model the simulation from DPAI and FE for the rectangular domain **(a)** and irregular geometry shape in **(b)**, respectively.*

anticipated simulation from the DPAI model in the bottom row. The suggested DPAI model is trained with boundaries that have straight edges, but it can produce simulations with irregular. The DPAI model is capable of producing reflection wave propagation from sharp edges as it has learned wave interaction physics at the domain edges from the training datasets. Thus, the DPAI model matches the FE and correctly predicts the propagation of reflection waves from the side and back walls.

4.3 Simulating Phased Array Beam Steering Wave Propagation Simulations using DPAI:

The third DPAI model is trained using the dataset generated by modelling the phased array beam steering simulations in FE simulations. We employ the same DPAI architecture as section 4.1. Using NVIDIA GeForce RTX 3090 GPU processors, the DPAI model is trained for minimizing the mean square loss function by back-propagation through time (BPTT) at a linear rate of 0.0001 over 300 epochs. The training procedure takes around 56 hours. As seen in *Figure 7(b),* the testing loss is calculated to be 0.00025, and the average training loss is 0.00078. The FE simulation dataset is used to evaluate the trained DPAI model in order to quantify its efficiency.

We have taken into consideration a variety of phased array beam steering simulations aside from the ones utilized during training and testing in order to evaluate the trained DPAI model qualitatively. The DPAI model receives the preceding 10 frames as input and outputs the next 5 frames to create the full simulations. This procedure loops up to the entire number of sequences of frames produced in a series. The initial frames obtained from the FE simulation are given as input for the first iteration of the simulation-generating process. The output of the previous iteration's generated frames is used as input in the subsequent iteration to complete the full-length simulations.

With the phased array beam steering angle set to 30 degrees, *Figure 8* depicts the wave propagation sequence of frames at the same time occurrences between DPAI and FE. In particular, we present the FE and DPAI simulation at exact time instances t = [0.9 μs, 1.1 μs, 1.5 μs, 1.9 μs, 2.2 μs] for the long-term simulation. The top row in *Figure 8* shows the FE (ground truth) sequence, while the bottom row reports the DPAI simulation. It is evident that there is a robust qualitative agreement between the DPAI-generated simulations and the FE simulations.

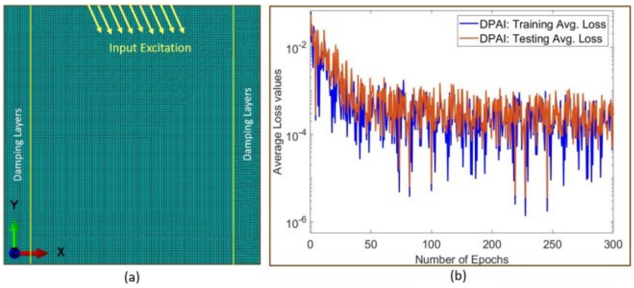


***Figure** 7: **(a)** FE modeling: all the active aperture elements are triggered in parallel using pre-defined delay laws to form the ultrasound beamforming to steer in the medium. **(b)** DPAI: Training/Testing: the average loss values over a number of epochs for phased array beam steering datasets.*

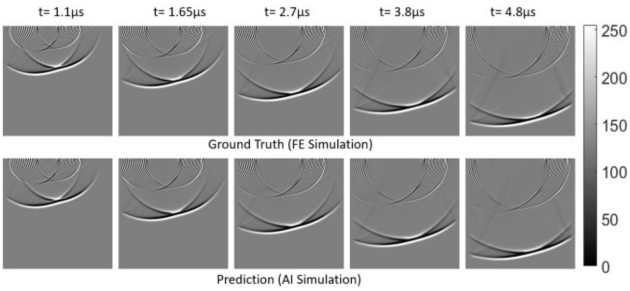


***Figure 8:** Phased array beam steering simulation*

The DPAI model performance in simulating the phased array beam steering simulation is compared with FE. In FE, a 16-element active aperture is used for generating simulation with the central frequency of 5 MHz with two cycles. The 30-degree beam steering pre-calculated focal law is applied in FE. The FE generated in the first 10-frames is fed to DPAI for generating successive next 5-frames.

The phased array (PA) ultrasonic technology allows for beam steering and focusing without requiring the transducer to move physically, it is the most advanced method for defect characterization and identification in the NDE domain. The main benefit of the PA technique over the traditional ultrasonic technique is that it is much faster to inspect large regions from a single location using a variety of ultrasonic profiles, such as beam and plane wave steering and focusing, without having to move the transducer.

5 CONCLUSION:

This work presents a novel and innovative deep learning DPAI approach for rapid computation of the ultrasonic wave propagation for point sources, reflection from boundaries, and phased array beam steering simulations. The method is trained using spatial-temporal FE simulation data. The DPAI model is learning representations of time-domain elastodynamic simulations from training datasets. In order to simulate the propagation of ultrasonic waves, data-driven, physics-aware AI prediction algorithms are used. A DPAI model is significantly faster than a conventional FE solver in computing simulation. The trained DPAI model enables users to simulate significantly larger domain simulations, single to multiple excitations point sources, reflection from irregular geometrical boundaries, and phased array beam steering ultrasonic wave propagation in 2D. The data it yielded demonstrated the suggested DPAI's efficacy in accurately replicating wave propagation phenomena. In this article, we first trained the AI network only by simulation of the wave transmission phenomena, and we were able to obtain the expected outcomes for the wave dynamics assessment for forward and reflection from boundaries. In further research, we will place many defect classes and their combinations to mimic different wave propagation scenarios, such as reflection, refraction, creeping, and scattering effects.

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