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Domain Decomposition Based Artificial Neural Networks (ANNs) Modeling of Acoustic Wave Resonators and Filters

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***Abstract*—This paper investigates the effectiveness of artificial neural networks (ANNs) as a surrogate modeling method based on machine learning algorithms in emulating the electroacoustic wave behavior of the high-*Q* piezoelectric resonators and filters. A domain decomposition approach incorporating ANN models to concurrently analyze multidomain radio frequency (RF) modules is also discussed. Different multilayer perceptron (MLP) ANN models have been developed and benchmarked against their model accuracy and model efficiency. The developed models are then utilized to construct ladder-type Band 7 and Band 41 bandpass transmit filters, as examples, to highlight the quality of the modeling method. Other possible applications pertinent to the capability of machine learning algorithms are briefly discussed.**

Keywords*—Acoustic wave (AW) resonator, artificial neural networks (ANNs), bandpass, ladder-type filters, device modeling, domain decomposition, machine learning.

I. Introduction

In the recent years, surrogate models based on machine learning algorithms have gained a great attention as alternative to physics-based models and simulations for their efficient model utilization, accuracy, suitability for automatic model creation, and versatility since they are not limited to specific structures [1-6]. Behavioral or black-box models based on artificial neural networks (ANNs) can learn the input-output relationship of a given system or a device as well as performing pattern recognition using as little training data and user interaction as possible. ANN modeling facilitates accurate and fast models of realistic technology modification scenarios where training data is expensive or sparse. In addition to the conventional MLP ANN, several advanced ANN structures have been explored in the literature such as recurrent neural networks (RNN) where feedback loops allow information to be stored within the network to perform complicated tasks [2, 3], and reverse-modeling using knowledge-based ANN (KBNN) where the input-output variables are reversed in a systematic manner to improve the model accuracy. Such complex ANN topologies can be utilized when standard MLP ANN fails to deliver a satisfactory performance [4]. The study proposed in this paper uses conventional ANN structure which are found to be of sufficient accuracy to model the acoustic-wave (AW) resonator behavior, as will be demonstrated in Section III.

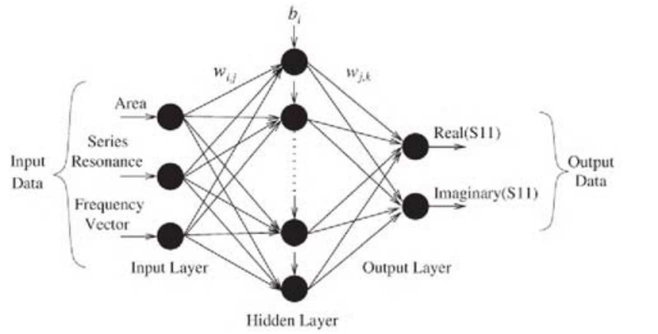


Fig. 1. Representation a conventional MLP feedforward neural network consisting of 3-layers (a layer of three inputs, a single hidden-layer of *N* neurons, and a layer of two outputs).

Fig. 1 is an illustrative example of an ANN model with specific AW resonator input/output design parameters. *w* and *b* are both adjustable scalar parameters for each neuron and governed by the training algorithm in use.

Efficient design and analysis of multidomain packaged devices and radio frequency front-end (RFFE) modules is a key to the development of competitive communication pruducts by ensuring their reliability and by accelerating the product time-to-market. Attempting to emulate the complexity of such systems by incorporating all degrees of freedom using brute-force simulation methods requires an extremely large computational overhead which hinders the ability to carry out accurate and efficient system-level analysis. Alternatively, domain decomposition methods based on cascading models from different domains (e.g., mechanical, acoustical, electrical, and/or thermal domains) have been widely adopted in the microelectronics industry for the analysis of multidomain modules. Such schemes allow concurrent system-level analysis and improve the product re-design cycles.

The intent of this work is to develop machine learning based models which can accurately and efficiently emulate the behavior of AW resonators. The developed models will then be utilized to construct ladder-type bandpass filters to benchmark the model accuracy. AW devices find several applications in RFFE modules especially for portable wireless systems where small size, light weight, and high performance are paramount.

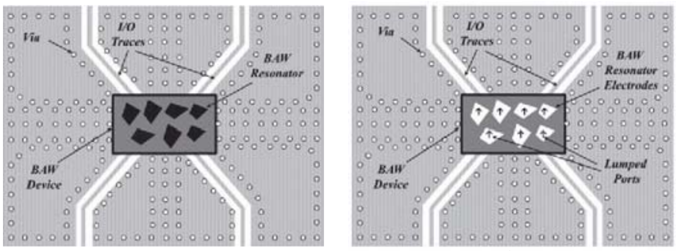
II. Modeling Approach

A. Domain Decomposition

Available standalone simulation tools are limited in terms of their capability to perform multi-domain analysis. For example, typical computational electromagnetic (CEM) tools are incapable of analyzing nonlinear and digital devices. On the other hand, multiphysics based solvers are computationally expensive and therefore inefficient in handling large design optimization problems. Understanding these challenges and trying to thoroughly emulate the complexity of modern RF modules has led to developing several modeling approaches that can facilitate system-level analysis and optimization. Among these methods, domain decomposition schemes are the most commonly used allowing fast-paced product development cycles and, as a result, shorter product time-to-market.

In the analysis of electroacoustic wave devices, the performance is evaluated by incorporating models from the two separate domains, electromagnetic and electroacoustic, which are then simulated concurrently via a circuit solver tool. The electromagnetic (EM) model is required to capture the EM parasitics from the package housing the acoustic components, while the electroacoustic model is necessary to describe the behavior of the piezoelectric components in the device. This approach offers an efficient, yet accurate and concurrent analysis for evaluating and optimizing complex RF systems.

Fig. 2 illustrates a co-design approach based on domain decomposition. Here, the linear domain (die packages, PCB traces, embedded passives, evaluation board, etc.) is analyzed by a CEM tool to extract their network parameters (e.g., S-matrix). An S-parameter matrix can then be imported into a circuit simulator (e.g., Keysight ADS) to link into it nonlinear (or electroacoustic) surrogate models enabling a concurrent multi-domain analysis. It is worth pointing out that the frequency dependent nature of the linear domain (device package) requires that the network-parameters are computed at the frequency band of interest; thus, dispersion characteristics are well-preserved.



(a) (b)

Fig. 2. A domain decomposition example of an electroacoustic packaged filter mounted on an evaluation board: (a) a full model containing both the piezoelectric (nonlinear-domain) and packaging (linear-domain) materials; and (b) the model-problem in (a), however, with lumped ports replacing the piezoelectric material (i.e., to model the linear domain only).

B. Machine Learning Based Modeling

Machine learning methods are typically classified into supervised learning where input/output data are available for modeling, and unsupervised learning where only input data is known (e.g., pattern recognition) [7]. ANNs among others are the most prominent machine learning method as they are flexible, scalable, and exhibit exceptional generalization and extrapolation capabilities. In addition, ANN models can efficiently handle complex optimization problems, especially when dealing with a multidimensional modeling space that requires covering wide parametric sweeps, emulating highly nonlinear device behaviors, and dealing with high-Q resonances. All these benefits broaden the scope of their application. According to the Universal Approximation Theorem [8], a three-layer MLP ANN structure can approximate any arbitrary nonlinear, continuous, and multi-dimensional input-output function to any level of desired accuracy.

A machine learning algorithm uses computational methods to train the model directly from input data without relying on empirical, analytical, or physics-based models. Assume x represent an m-vector, containing physical or geometrical input model parameters (e.g., area or static capacitance, series resonance frequency, etc.) of an AW resonator, and let y represent an n-vector containing the output model responses (e.g., real and imaginary parts of S_{11}). The relationship between y and x can be described as $y = f(x)$, where f represents a detailed physics-based model. The ANN model for such relationship can be represented as $y = f_{\text{ann}}(x, w, b)$, where w is a weight vector and b is a bias vector of the neurons that are iteratively adjusted during the network training process so as to minimize the training error. Among many other error functions, mean squared error (MSE) is the most common measure for regression. MSE calculates the average squared difference between the modeled outputs and the exact outputs. Training data critical to the development of the ANN models can be acquired through high fidelity finite element method simulations or measurements. Training data are usually normalized at the input layer to facilitate the training process. In fact, data normalization is an important step since the input parameters may include input vectors with large element values and other vectors with small element values that may also differ from one modeling problem to another by orders of magnitude. This, in turn, could affect the learning quality as the output values may become sensitive to the input values with higher magnitude. MLP ANN algorithms are typically trained using backpropagation methods (i.e., starting from the output layer and propagate backwards) to update its weights based on the pre-defined error function. Generally, as the number of samples available for training increases, the modeling accuracy increases.

The activation function of the neurons in the input layer is a relay function (i.e., no computation is performed at this layer), while for the output neurons it is a linear function that computes the weighted sum of the inputs of the output neurons. The activation function of the hidden layer can be one or a combination of several functions such as sigmoid, arc-tangent, or hyperbolic tangent [6]. The sigmoid function is commonly used and given by

$$\sigma(\gamma) = \frac{1}{1 + e^{-\gamma}} \tag{1}$$

where γ and σ are the input and output of the hidden neuron, respectively. The sigmoid function is bounded, continuous, monotonic, and differentiable (i.e., the slope of the sigmoid curve can be determined at any two points). The function exists between 0 to 1, which is applicable for problems that deal with probability prediction and output data that is known to lie within

TABLE I. PARAMETERS OF THE DEVELOPED SINGLE LAYER AW RESONATOR-LEVEL ANN MODELS

LTE Frequency Band	ANN Model	Number of Neurons	Number of Epoch	Training Algorithm	Mean Squared Error (MSE)	Size of Training Data	Size of Validation Data	Size of Testing Data	Resonator Input Design Parameters		
									Area (μm^2)	Series Resonance (MHz)	Frequency Vector (MHz)
Band 7	Series Resonator	150	1000	Levenberg–Marquardt	1.945e-06	50434	10807	10807	7000 – 12000 (1000 μm^2 step)	2538 – 2552 (2 MHz step)	1500 – 3000 (1 MHz step)
				Scaled Conjugate Gradient	1.090e-03						
				Bayesian Regularization	5.101e-07						
	Shunt Resonator	150	1000	Levenberg–Marquardt	6.459e-07	50434	10807	10807	20000 – 25000 (1000 μm^2 step)	2458 – 2472 (2 MHz step)	
				Scaled Conjugate Gradient	2.671e-3						
				Bayesian Regularization	1.332e-07						
Band 41	Series Resonator	150	1000	Bayesian Regularization	1.452e-07	69346	14860	14860	9000 – 19000 (2000 μm^2 step)	2600 – 2700 (10 MHz step)	1000 – 4000 (2 MHz step)
	Shunt Resonator	150	1000	Bayesian Regularization	2.464e-07	69346	14860	14860	9000 – 19000 (2000 μm^2 step)	2450 – 2550 (10 MHz step)	

certain value bounds. The purpose of the activation function is to introduce nonlinear functionality to the neurons being trained.

It is worth pointing out that complex valued data must be split into two components, (real and imaginary) or (magnitude and phase), when they are used as output vectors. In addition, one may want to examine different equivalent network parameters (*Z*-, *Y*-, or *S*-parameters) of the data being modeled to determine which waveform results in fewer discontinuities to facilitate the machine learning process.

III. RESULTS AND DISCUSSION

An AW ladder filter comprises series and shunt resonators. Considering the ANN model for an AW resonator with input/output design parameter as illustrated in Fig. 1, four sets of ANN models have been developed with the aid of MATLAB [7]. Two models for the series and shunt resonators of Band 7, respectively. Similarly, another two models for the series and shunt resonators of Band 41. The input design space for the two filters are described in Table I. Data required for the development of the ANN models are based on de-embedded measured on-wafer resonator data.

Three different ANN training algorithms have been evaluated (Levenberg-Marquardt, Bayesian Regularization, and scaled conjugate gradient) which are suitable for function approximation problems. The Bayesian Regularization algorithm can provide excellent correlation to the data being modeled at a relatively slower convergence rate when compared to the other two algorithms. The conjugate gradient algorithm has the fastest convergence and requires less computational resources; however, it has the least model accuracy for the same number of epochs and a given number of neurons. All three algorithms are used to train feedforward ANN networks where the information propagate only in one direction. This is different from a recurrent ANN that incorporates feedback loops.

The number of neurons required for producing accurate ANN model has been determined in a trial error fashion by gradually increasing the number of neurons and comparing the MSE of the generated models. In this study, 15% of the available samples are used for validation and another 15% are used for testing the final/generated ANN model while the remaining 70% of the data are used for training. Both testing and validation datasets are used to provide unbiased evaluation of the model accuracy. While the testing dataset is an objective measure used to gauge the accuracy of the final model once it is completely trained, the validation dataset is utilized to frequently evaluate and tune the model during the training process (however, it doesn't participate in the training process in any way).

After the successful development of the ANN AW resonator models, Band 7 and Band 41 ladder-type filters were constructed and compared against the exact performance as demonstrated in Fig. 3. The exact performance is based on de-embedded measured resonator data that were used to construct the filters response in a circuit schematic level.

It was observed that a small number of neurons (40 neurons) were adequate to provide accurate prediction of the filter's out-of-band (OOB) rejection performance, while a larger number of neurons was needed to accurately mimic the in-band behavior (i.e., insertion loss and impedance shape).

The results, given in Table I, show high accuracy of the generated ANN models using the Bayesian Regularization training algorithm as demonstrated with the Band 7 case study. Consequently, the same algorithm was applied to model the Band 41 resonators. Although the input design parameters are well spaced in Band 41 data when compared to the Band 7 data, the generated model resulted in a relatively similar accuracy level.

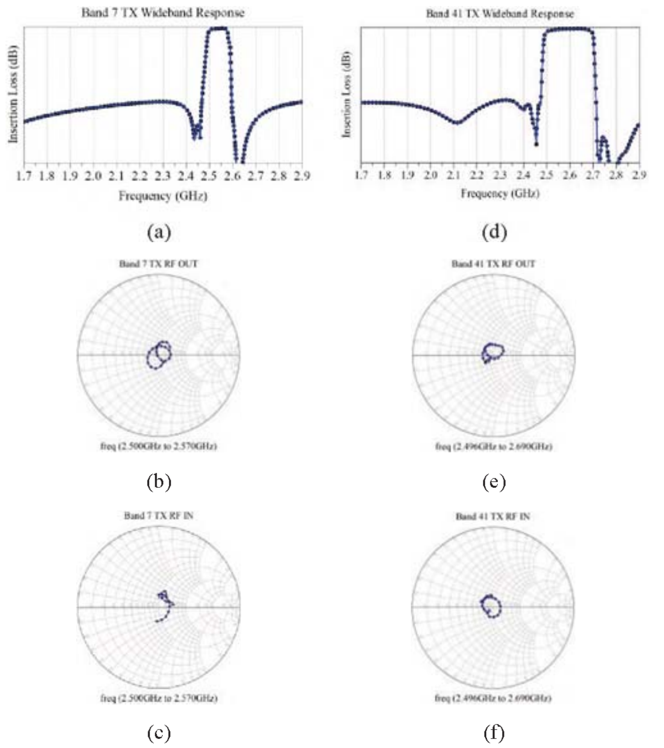


Fig. 3. Modeled (blue solid line) and exact (black circular symbols) performance. (a); (b); and (c) Band 7 wideband; input; and output reflection coefficient, respectively. (d); (e); and (f) Band 41 wideband; input; and output reflection coefficient, respectively.

IV. Potential Applications

Other possible applications that could utilize the capabilities of machine learning algorithms in the field of AW filters design include:

A. Die Layout Optimization

One of the time-consuming steps in the design process of an AW filter is the preparation of the die layout. Generally, the resonators in a packaged filter layout need to be arranged in a way that avoids EM parasitic coupling among the resonators themselves and with the filter package. Additionally, the layout must be designed so that it has the least routing loss between the input and the output of the filter. Machine learning algorithms can be trained to provide the proper arrangement of resonators for a given package size, filter topology, and number of resonators.

B. BAW Resonator Pattern Recognition

Apodization is the process of modifying the lateral structures of a bulk acoustic wave (BAW) resonator for spurious mode suppression. ANN can be trained to learn the resonator patterns for a given BAW stack that results in the least possible spurious distortion. A modeling scenario may include input parameters such as the rectangular coordinates of the resonator's electrodes (e.g., polygon vertices) over a sweep of frequency, while the output could be a measurement equation to identify the occurrence of the spurious modes (e.g., sharp slopes in response) outside the series and parallel resonances of the BAW resonator.

C. Automatic Model Extraction

AW resonator surrogate models can be developed by automating the sample selection of the ANN training data which are usually computationally or experimentally expensive. This can be accomplished by driving a FEM simulation solver or an on-wafer measurement setup to only select the necessary data points for training that ensure a user predefined model accuracy. A highly adaptive sampling algorithm (e.g., Lola-Voronoi [9]) is typically used for this purpose to balance the data selection process between dividing the design space into equally spaced points and selecting more points in highly nonlinear regions.

V. Conclusion

In this study, three different machine learning algorithms employing ANNs have been developed and benchmarked to model the behavior of AW resonators. The successfully developed models are utilized to construct Band 7 and Band 41 transmit ladder-type bandpass filters which are then compared against the exact filter response. Among the three training algorithms, it was observed that the Bayesian Regularization method provides the least MSE and yields accurate model prediction. It is worth mentioning that the developed ANN models can be easily incorporated into a circuit solver as custom nonlinear equation-based components (e.g., as Keysight ADS symbolically-defined device, SDD).

Several potential applications that could benefit from the capabilities of machine learning algorithms are discussed and summarized in this paper. Additionally, artificial intelligence (AI) based algorithms are expected to have vast deployment in the foreseeable future wireless communication technologies as in the new fifth generation (5G) mobile networks.

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