## Imperial College London

## Department of Earth Science and Engineering

## MSc in Applied Computational Science and Engineering

## Independent Research Project

## Project Plan

Using Machine Learning Approach to Simulate Wave Propagation in Solids

by

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# Introduction

Wave propagation problems have been of concerns for a long time in different engineering areas. The use of materials and structure designs need to take earthquake damage into account []; the detection of certain mines depends on the characterisation of corresponding features by scanning the subsurface via seismic wave tomography []; ultrasonic waves are used in damage detection and diagnosis []. Partial differential equations (PDEs) in simple and computationally cheap wave propagation problems could be solved analytically; However, when the problem is complicated, either a specific analytical solution does not exist, or the computation cost would be extremely high.

Numerical solutions, therefore, have been the dominant solution for wave propagation problems. Depending on specific problems aimed to address, different strategies have been developed. The most widely used methods are *Finite difference method* (FDM) and *finite element method* (FEM). FDM solves differential equations by approximating the derivatives at the user-defined spatial resolution and is easy to be developed into high-order in space, The use of FDM is limited due to its inability to address unstructured mesh, though (Li et al., 2020; Lahivaara et al., 2018). *Finite element method* (FEM) is the most commonly used method in various engineering applications thanks to its ability for meshing the arbitrary domain. Previous work has used FEM to analyse ultrasonic waves in heterogeneous media in 2D (Freed et al., 2016; Lhuillier et al., 2016; Nakahata et al., 2016) and elastic waves in 3D (Van Pamel et al., 2015; Van Pamel et al., 2017). Other methods have also been studied for specific problems considering their physical features. *Discrete element method* (DEM), instead of generating arbitrary mesh shapes in the domain, assumes the material already to be particle-like and discretely distributed which has been used to investigate propagation patterns (Gu and Yang, 2018), wave frequencies (O’Donovan et al., 2016) and energy dissipation (Ning et al., 2015). Given the discrete nature, however, DEM is mostly used for granular media which limits its generalization ability. *Finite Volume Method* (FVM) evaluates volume integrals as fluxes and solves the partial differential equations (PDE) by balancing the input and output fluxes. FVM was found to have in increase in accuracy comparing to other reference methods for both isotropic and complex media in 2D and 3D simulation (Dumbser et al., 2006). *Method of fundamental solutions* (MFS) is a mesh-free method which approximate solution of boundary value problems for homogeneous PDEs which seems promising to represent complex reflection and refraction patterns for distinctly separated materials (Nennig et al., 2012).

However, when it comes to a complicated problem, numerical methods, although guarantee the quality of the analysis, could require heavy costs of computational resources (Kononenko et al., 2018). By contrast, machine learning-based methods, particularly neural networks, have benefitted from recent years’ improvement of computational capabilities. Neural networks regard problems as a collection of information and try to “learn” and hence solve it by exploring the internal statistical and mathematical correlations. The initiative of the machine learning approach for engineering problems in solids generally falls into two aspects: (1) to develop an architecture that out-speed numerical solutions (Zhu et al., 2017) and (2) to re-use the learnt network for transferring learning (Kononenko et al., 2018). Various architectures have been developed in different areas. Convolutional autoencoders were developed to adapt arbitrary aorta shapes from real patients and generate the stress distribution (Liang et al., 2018), some for the purpose of valve design (Liang et al., 2017; Aranda et al., 2018; Balu et al., 2019); Bai et al. (2018) used a multi-scaled fully convolutional neural network (CNN) to automate the diagnosis for cardiovascular diseases; Nie et al. (2020) predicted the stress field for cantilevered structures using an in-between architecture combining two CNNs and took multi-layered images as input. Additionally, one crucial feature of neural networks is that it addresses realistic problems without the need to know background equations i.e. learn by “basic physical instinct” like human (Lahivaara et al., 2018; Zhu et al., 2017).

Numerical solutions for wave propagation problems also suffer from the expensive computational cost and calculation time. A group of architectures have been developed. Zhu et al. (2017) developed a generative adversarial network (GAN) to simulate various wave sources to simulate wave dynamics in 2D. They found a multi-scaled generator is able to generate accurate results for both homogeneous and heterogeneous media with only 720 training datasets, the GAN itself suffered from exploding generator loss at late steps, though. Sorteberg et al. (2018) developed a convolutional recursive neural network (RNN) with long short-term memory (LSTM) to predict the wave front patterns within a homogeneous 2D domain, where the result shows good fit at first and had diverged at 24th step. Lahivaara et al. (2018) used an AlexNet-based (Krizhevsky et al., 2012) CNN to characterise properties such as tortuosity and porosity of a solid surrounding by the liquids from FEM-generated incidence images. Neural networks have been especially popular for fault detection and crack diagnosis. Li et al. (2019) developed an autoencoder based on U-Net (Ronneberger et al., 2015) to generate predicted fracture image by training 2D-seismic sections; Sbarufatti et al. (2014) used a numerically enhanced artificial neural network (ANN) to generate fracture positions and angles using FDM-based results validated by the baseline data from experiments. More methods using deep residual network (ResNet) and GAN has been summarized by Jiao et al. (2020).

Generally, wave propagation problems in the engineering field is crucial for understanding material and structure features which can be applied into practices. However, the large simulation demand and short time-being requirements have urged researchers to explore alternative solutions to the conventional numerical methods. At the fast pace of development of computational capabilities, solving wave propagation problems using neural network models have received promising results from previous work, yet given that most of the papers were published within three years, there is still a huge space for new explorations into it.

# Project Plan and Justifications

The project will focus on the exploration of neural networks for solving wave propagation problems. It will include four steps: (1) generating wave propagation data from numerical solutions, (2) developing a neural network architecture for the specified problem, (3) training and validating the neural network and (4) post processing. The project will generally follow the process of Figure 1.



Figure 1 Proposed workflow of the project.

As shown in Figure 1, the workflow starts from generating data from numerical models. Thus, the selection of an appropriate tool is crucial for generating high-quality input data to feed the neural network. Most of the studies reviewed earlier have chosen FEM for its flexibility and large occupation in the engineering tool market, e.g. ANSYS and ABAQUS, etc. This project will follow the mainstream and utilise this publicly acknowledged solution. However, the selection of tools is restricted by the limited resources for the project; therefore, ANSYS Student Edition will be used as an open-source tool as a compromise.

Table 1 Timing comparison between a square and a cube.

|  |  |  |  |
| --- | --- | --- | --- |
| Square | 10x10 mm2 | 80x80 mm2 | 80x80 mm2 |
| Element Size/mm | *1* | *1* | *0.6* |
| Node No. | *121* | *6561* | *17956* |
| Time | *6.3* | *9.6* | *9.45* |

|  |  |  |
| --- | --- | --- |
| Cube | 10x10x10 mm2 | 80x80x80 mm2 |
| Element Size/mm | *1* | *3* |
| Node No. | *1331* | *21952* |
| Time | *6.7* | *13.5* |

*Previous work showed that wave propagation-related studies mostly focused on 2D and 3D problems. However, full 3D models have remained scarce in seismology and non-destructive evaluation (NDE) even with numerical solutions (Pamel et al., 2017), not to mention neural networks which just began to gain attention in the engineering academia. The only material reviewed trying to train a model that accepts 3D geometries is not related to wave propagation (Gao et al., 2020). Additionally, a basic experiment was done for ANSYS Student Edition to compare the approximating time consumption regarding 2D and 3D problems. Timings for the two geometries are summarised in Table 1. It appears that for coarsely discretised domain the difference is rather small; however, when the element number increases to 102, a significant 42% increase of time use is shown for 3D geometry. The approximated size of the dataset, according to reviewed papers, falls within the range of 103 – 105 which means an additional ~104 – 106s is needed for 3D problems, if finely discretised. Thus, this project will focus on 2D problems rather than 3D, given the tight schedule and the possibility for 2D simulation to provide much finer results.*

Wave propagation problem falls into different parts. In reviewed literatures, the background initiative could be non-destructive evaluation, material characterisation and wave dynamic simulations (Zhu et al., 2017; Li et al., 2019; Sbarufatti et al., 2014). The NDE example, however, was assisted by the baseline data from experiments, whereas the material characterisation could be interpreted as a derived application from pure wave dynamic simulations. Thus, this project will focus on the wave dynamics and its propagating properties in a domain for an intuitive development of a new neural network to be compared with previous work. Therefore, the current design of the project would be generating data from the ANSYS simulator to provide a 2D multi-coloured image as training and validation data. Hence, the project will concentrate on the development and study of a CNN as a new solution to wave propagation problems.

A screenshot of a social media post

Description automatically generated

Figure 2 Gantt chart for the project.

development of the network architecture could cost longer than the assigned period; if so, The Gantt chart is therefore scheduled for the project (Figure 2). Some risks worth discussion and backup plans will be provided as a compromise. In Developing Network stage, the actual the time spent on generating new data will be shortened to meet the proposed starting date of post-processing stage. If unforeseeable drawback happened and caused unavoidable delay to start the last stage, the first task in the Post-processing and Report Writing stage will be cancelled to meet the deadline for submission. The chart is subject to continuing alterations dependent on the progress and results in each step.

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