## Imperial College London

## Department of Earth Science and Engineering

## MSc in Applied Computational Science and Engineering

## Independent Research Project

## Project Plan

Developing Neural Networks to Simulate Wave Propagation in Solids

by

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# Introduction

Wave propagation problems have been a concern in various engineering areas, e.g. structural analysis (Nie et al., 2020) and material property characterization (Lahivaara et al., 2018). Seismic wave propagation damage needs to be evaluated before a pipeline system to be installed (O’Rourke et al., 1993); ultrasonic wave was used in determining gasoline volatility characteristics by measuring the wave velocity (Takahashi et al., 2000); lamb wave sensing network was used in aluminum skin structural health monitoring (Sbarufatti et al., 2014).

Wave propagation through materials is described using a partial differential equations (PDE). When an analytical solution is known for a specific problem, it can be solved directly; however, in the real-world wave propagation problems, the solution is likely to be unknown and, therefore, numerical solutions, which offer a way to obtain acceptable simulation results, have been dominant in solving wave propagation problems. Different strategies have been developed for specific problems. 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 easily developed into high-order in space but limited due to its inability to address unstructured mesh (Nie et al., 2020; Lahivaara et al., 2018). FEM is the most commonly used method thanks to its ability for meshing the arbitrary domain and the capturing local effects by the mesh refinement (Reddy, 2006). Previous work 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: *discrete element method* (DEM) has been used to investigate propagation patterns for micro-scale domains (Gu and Yang, 2018), wave frequencies (O’Donovan et al., 2016) and energy dissipation (Ning et al., 2015) for particle-like media and incident boundary patterns for joint-mass rocks (Fan et al., 2004). *Finite Volume Method* (FVM) evaluates volume integrals as fluxes on the finite volume boundary and solves the partial differential equations (PDE) by balancing the input and output fluxes (Fallah et al., 2000). Dumbser et al., (2006) found FVM can provide accuracy comparable to other reference method, e.g. FEM, for both isotropic and complex media in 2D and 3D simulation. *Method of fundamental solutions* (MFS) is a mesh-free method which approximates the solution of boundary value problems for homogeneous PDEs which is promising to represent complex reflection and refraction patterns for distinctly separated materials (Nennig et al., 2012).

However, numerical methods could be computationally expensive for complex problems (Kononenko et al., 2018; Zhu et al., 2017). By contrast, neural networks (NN) have benefitted from recent years’ improvement of computational capabilities. One advantage of NN is it requires no underlying physical formula in advance, meaning the computational consumption depends only on its architecture (Zhu et al., 2017; Kononenko et al., 2018). Various NN architectures have been developed in different areas. Convolutional autoencoders were developed to adapt arbitrary aorta shapes and generate the stress distribution (Liang et al., 2018) and valve design (Aranda et al., 2018; Balu et al., 2019); Nie et al. (2020) predicted the stress field for cantilevered structures using an in-between architecture combining two CNNs which took multi-layered images as input.

A group of NNs have been developed for wave propagation problems based on popular architectures including generative adversarial network (GAN), CNN and recursive NN (RNN). Zhu et al. (2017) developed a 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 generated from an FDM-based simulator (CIG, 2019), the GAN itself suffered from the exploding generator loss, soaring to 1x103 at 2x105 iterations, though. Sorteberg et al. (2018) developed a convolutional RNN with long short-term memory (LSTM) to predict wave front patterns within a homogeneous 2D domain, where the result showed good fit at first and diverged at 24th step. Lahivaara et al. (2018) used an AlexNet-based (Krizhevsky et al., 2012) CNN to characterise solid properties including tortuosity and porosity on sensor points for an unknown solid surrounded by water from FEM-generated incidence images. NNs have been regularly used for fault detection in earthquake scale and crack diagnosis for small-scale engineered materials. Li et al. (2019) developed a U-Net-based (Ronneberger et al., 2015) autoencoder to generate predicted fracture image by training 2D-seismic sections; Sbarufatti et al. (2014) used a numerically enhanced artificial NN to generate fracture positions and angles using FDM-based results. More methods using CNN and GANs have been summarized by Jiao et al. (2020).

Generally, wave propagation problems in the mechanical engineering and bioengineering fields are crucial for understanding material properties and structural weaknesses, etc. However, the large simulation demand has urged researchers to explore alternative solutions to the conventional numerical methods. With developed computational capacity, solving wave propagation problems using NNs has received promising results from previous work.

# Project Plan and Justifications

*Overview:* Based on the literature review discussed earlier, the project will focus on the use of NNs for solving wave propagation problems. Key decision steps will be discussed in this section. The project will follow the process of Figure 1 and the time schedule of Figure 2.



Figure 1 Proposed workflow of the project.

*Generating wave propagation data from numerical solutions:* 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 NN. Most of the studies (Lahivaara et al., 2018; Nie et al., 2020; Sbarufatti et al., 2014) reviewed earlier have chosen FEM for its flexibility and large occupation in the engineering tool market, e.g. ANSYS and ABAQUS, etc. 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* |

*Choosing to simulate a 2D domain:* This project will focus on 2D problems. Previous work showed that wave propagation relating NN studies mostly focused on 2D problems. Quite a few NN structures mentioned above have been established for 2D (Zhu et al., 2017; Sorteberg et al., 2018; Lahivaara et al., 2018), which would enable performance comparisons with previous work (Fortiatis et al., 2020). By contrast, to the best of the author’s knowledge, only Gao et al. (2020) developed a CNN accepting 3D geometries for in situ stress prediction. A 3D NN could be stressing considering the re-design of cost function and re-formation of established 2D NN structures given the tight timeline. Additionally, a basic experiment was done using ANSYS Student Edition to compare the approximated time consumption for 2D and 3D problems. Timings for the two geometries are summarised in Table 1. It appears that when the node number increases to 105, 3D simulation requires 42% addition of time. The approximated dataset size from reviewed papers falls within the range of 103 – 105 which means an additional ~104 – 106s is needed for 3D problems, if finely discretised. ANSYS Student Edition also has a limit for 512k node number, which means for a 3D geometry fine mesh is not applicable.

*Specific wave propagation problem to be solved:* This project will focus more on the NN development. Choosing to solve 2D domain would offer a chance to finely mesh the domain so that subtle effects are more likely to be captured (Reddy et al., 2006). In this case, the project will solve a simple rectangle domain with a detonation point inside the domain to simulate a shock wave propagation pattern. Shock waves have been studied extensively due to its discontinuous feature of stress and strain and the loss of energy (Danilov et al., 2000; Hu et al., 2006). Among reviewed literatures, the author found a lack of studies in the shock wave simulation area using NNs, and therefore this project would be a guiding one if successfully implemented.

*Developing a NN architecture*: As far as the author has reviewed, the extensive use of CNN has received decent results with a training dataset ranging from very small (102, Zhu et al., 2017) to very large (105, Nie et al., 2020). The prevalence of image recognition also boosted the development of different CNNs designs including ResNet (Nie et al., 2020) which uses a residual network design, U-Net which is empowered by the multi-scaling design (Fotiadis et al., 2020), and Squeeze and Excitation blocks which enables channel-wise recalibration (Nie et al., 2020) . A method to combine available techniques is therefore interesting to be established and compared against existing ones. However, as previously reviewed literatures did not focus on shock waves, the performance of such a design is not guaranteed.

A screenshot of a cell phone

Description automatically generated

Figure Gantt chart for the project.

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