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

Hao Lu

hl1319@ic.ac.uk

GitHub login: acse-hl1319

Supervisor:

Dr. Adriana Paluszny

June 2020

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 1×10^3 at 2×10^5 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.

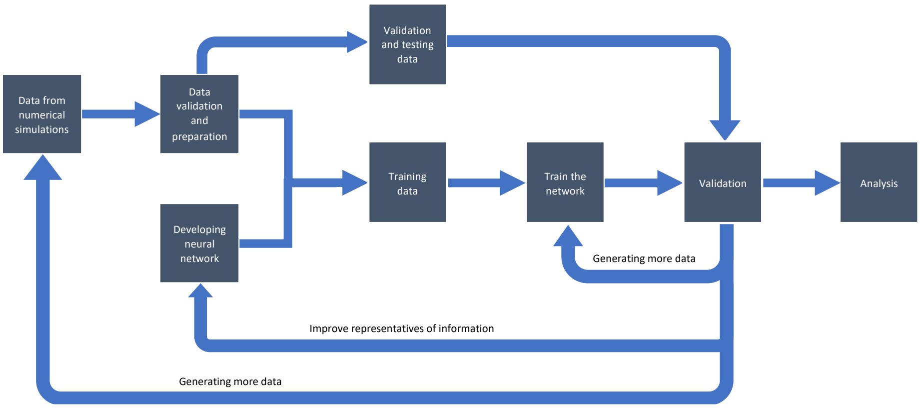

Figure 1 Proposed workflow of the project.

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 mm^2*	*80x80 mm^2*	*80x80 mm^2*
Element Size/mm	*1*	*1*	*0.6*
Node No.	*121*	*6561*	*17956*
Time	*6.3*	*9.6*	*9.45*

Cube	*10x10x10 mm^2*	*80x80x80 mm^2*
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 10^5, 3D simulation requires 42% addition of time. The approximated dataset size from reviewed papers falls within the range of $10^3 - 10^5$ which means an additional ~$10^4 - 10^6$s 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 (10^2, Zhu et al., 2017) to very large (10^5, 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.

Independent Research Project

Imperial College

Wave Propagation with Neural Network

Hao Lu

01/06/2020

1

TASK	PROGRESS	START	END
Preparation			
Design and justify project compositions	100%	1/6/20	26/6/20
Review wave propagation problems	100%	1/6/20	4/6/20
Review numerical methods for wave propagation problems	100%	5/6/20	12/6/20
Learn to automate ANSYS simulations	100%	8/6/20	26/6/20
Review relevant machine learning papers	100%	12/6/20	26/6/20
Finishing project plan	100%	15/6/20	26/6/20
Data simulation			
Develop and test scripts in ANSYS for shock wave propagations	0%	27/6/20	4/7/20
Generate a small group of data to discuss and validate	0%	1/7/20	6/7/20
Massively generate data	0%	7/7/20	10/7/20
Developing Network			
Analyse generated data and pre-processing	0%	11/7/20	14/7/20
Develop network architecture	0%	15/7/20	23/7/20
Train and validate network	0%	18/7/20	31/7/20
Re-generate data if needed	0%	24/7/20	31/7/20
Test network	0%	1/8/20	3/8/20
Post processing and writing the report			
Compare with training data visually	0%	4/8/20	7/8/20
Compare with training data mathematically	0%	8/8/20	11/8/20
Analyse and write the report	0%	11/8/20	23/8/20
Review the report and final check	0%	24/8/20	28/8/20
Insert new rows ABOVE this one			

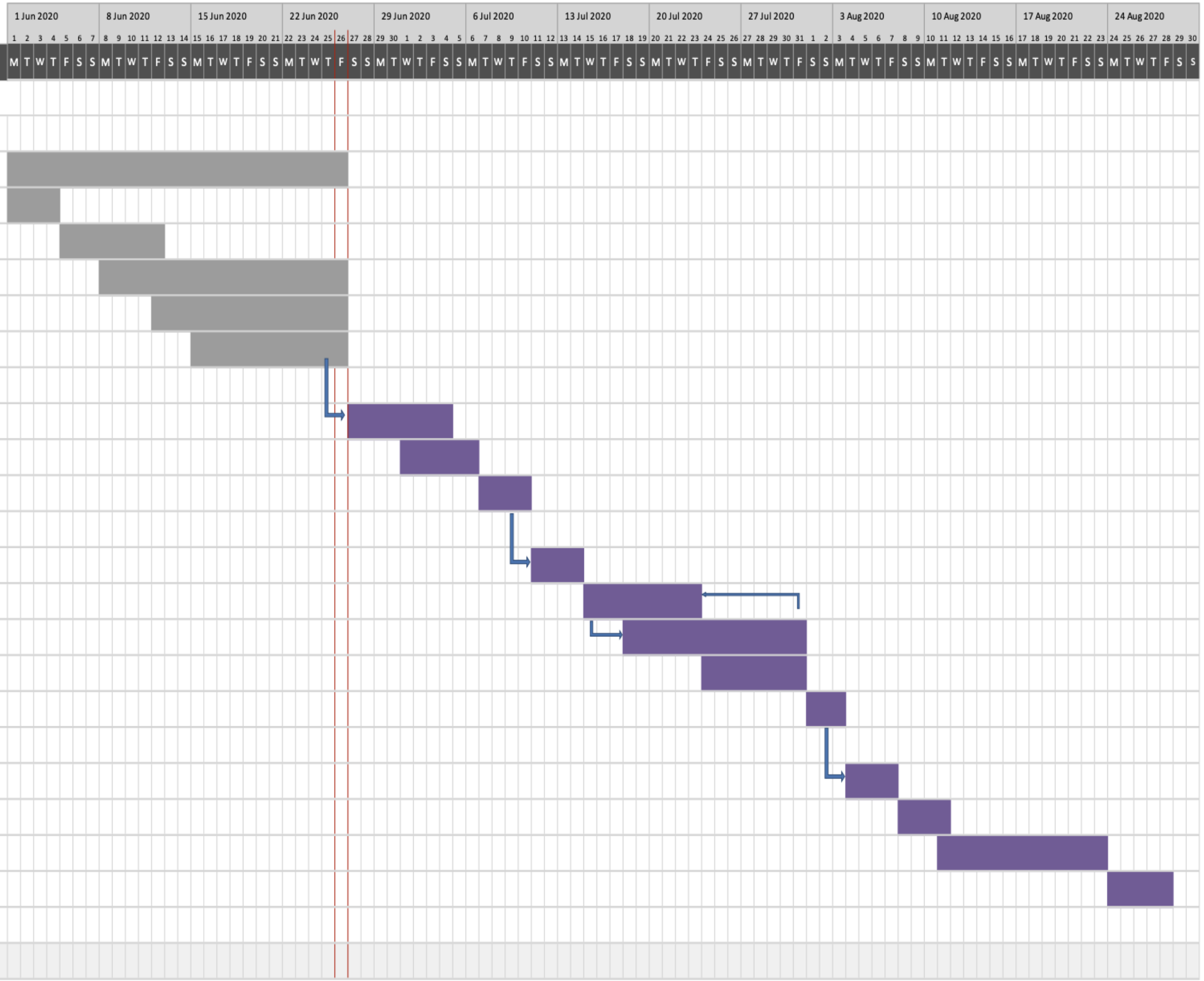

Figure 2 Gantt chart for the project.

Bibliography

1. Aranda, A. and Valencia, A., 2018. Study on cerebral aneurysms: Rupture risk prediction using geometrical parameters and wall shear stress with cfd and machine learning tools. Machine Learning and Applications: An International Journal (MLAIJ) Vol, 5.
2. Bai, W., 2018. Automated cardiovascular magnetic resonance image analysis with fully convolutional networks, 1–12. http://doi.org/10.1186/s12968-018-0471-x
3. Balu, A., Nallagonda, S., Xu, F., Krishnamurthy, A., Hsu, M.-C., & Sarkar, S., 2019. A Deep Learning Framework for Design and Analysis of Surgical Bioprosthetic Heart Valves. Scientific Reports, 1–12. http://doi.org/10.1038/s41598-019-54707-9
4. Carin, L., Geng, N., McClure, M., Sichina, J. and Nguyen, L., 1999. Ultra-wide-band synthetic-aperture radar for mine-field detection. IEEE Antennas and Propagation Magazine, 41(1), pp.18-33.
5. Computational Infrastructure for Geodynamics (CIG), 2019. Seismic_cpml. Accessed: 26/06/2020
6. Danilov, V.G. and Shelkovich, V.M., 2000. Propagation and interaction of shock waves of quasilinear equation. arXiv preprint math-ph/0012003.
7. Dumbser, M., Käser, M. and De La Puente, J., 2007. Arbitrary high-order finite volume schemes for seismic wave propagation on unstructured meshes in 2D and 3D. Geophysical Journal International, 171(2), pp.665-694.
8. Fallah, N.A., Bailey, C., Cross, M. and Taylor, G.A., 2000. Comparison of finite element and finite volume methods application in geometrically nonlinear stress analysis. Applied Mathematical Modelling, 24(7), pp.439-455.
9. Fan, S.C., Jiao, Y.Y. and Zhao, J., 2004. On modelling of incident boundary for wave propagation in jointed rock masses using discrete element method. Computers and Geotechnics, 31(1), pp.57-66.
10. Fotiadis, S., Pignatelli, E., Valencia, M.L., Cantwell, C., Storkey, A. and Bharath, A.A., 2020. Comparing recurrent and convolutional neural networks for predicting wave propagation. arXiv preprint arXiv:2002.08981.
11. Freed S, Blackshire J, Na J., 2016. Ultrasound finite element simulation sensitivity to anisotropic titanium microstructures. In Proc. of the Review of Progress in Quantitative NDE, Minneapolis, MN, 25–31 July 2015. Melville, NY: AIP Publishing.
12. Gao, D., Zhu, Y., Wang, X., Yan, K. and Hong, J., 2018, October. A fault diagnosis method of rolling bearing based on complex morlet CWT and CNN. In 2018 Prognostics and System Health Management Conference (PHM-Chongqing) (pp. 1101-1105). IEEE.
13. Gao, W., Lu, X., Peng, Y. and Wu, L., 2020. A Deep Learning Approach Replacing the Finite Difference Method for In Situ Stress Prediction. IEEE Access, 8, pp.44063-44074.
14. He, K., Zhang, X., Ren, S. and Sun, J., 2016. Deep residual learning for image recognition. In Proceedings of the IEEE conference on computer vision and pattern recognition (pp. 770-778).
15. Hu, Y., Yao, Z. and Hu, J., 2006. 3-D FEM simulation of laser shock processing. Surface and Coatings Technology, 201(3-4), pp.1426-1435.
16. Jiao, J., Zhao, M., Lin, J. and Liang, K., 2020. A comprehensive review on convolutional neural network in machine fault diagnosis. arXiv preprint arXiv:2002.07605.
17. Kononenko, O. and Kononenko, I., 2018. Machine learning and finite element method for physical systems modeling. arXiv preprint arXiv:1801.07337.
18. Krizhevsky, A., Sutskever, I. and Hinton, G.E., 2012. Imagenet classification with deep convolutional neural networks. In Advances in neural information processing systems (pp. 1097-1105).
19. Lähivaara, T., Kärkkäinen, L., Huttunen, J.M. and Hesthaven, J.S., 2018. Deep convolutional neural networks for estimating porous material parameters with ultrasound tomography. The Journal of the Acoustical Society of America, 143(2), pp.1148-1158.
20. Lhuillier P-E et al., 2016. Overview of the finite elements modeling of the ultrasonic propagation in complex media at EDF R&D. In Proc. 19th World Conf. on Non-Destructive Testing, Munich, Germany, 13–17 June 2016. See https://www.wcndt2016.com/Programme/show/Th-4-H-5.
21. Li, S., Yang, C., Sun, H. and Zhang, H., 2019. Seismic fault detection using an encoder–decoder convolutional neural network with a small training set. Journal of Geophysics and Engineering, 16(1), pp.175-189.
22. Liang, L., Liu, M., Martin, C., & Sun, W., 2018. A deep learning approach to estimate stress distribution: a fast and accurate surrogate of finite-element analysis. Journal of the Royal Society Interface, 15(138), 20170844–11. http://doi.org/10.1098/rsif.2017.0844
    Morlet CWT and CNN. In: Editor edito. Pub Place: IEEE. p. 1101-1105.
23. Nakahata K, Mizokami N., 2016. Image-based finite element simulation of ultrasonic wave in polycrystalline metal using phase-field modeling. In Proc. 19th World Conf. on Non-Destructive Testing, Munich, Germany, 13–17 June 2016. See https://www.wcndt2016.com/Programme/ show/Th- 3- H- 5.

24. Nennig, Benoit & Perrey-Debain, Emmanuel & Chazot, Jean-Daniel, 2011. The method of fundamental solutions for acoustic wave scattering by a single and a periodic array of poroelastic scatterers. Engineering Analysis with Boundary Elements. 35. 10.1016/j.enganabound.2011.03.007.
25. Nie, Z., Jiang, H. and Kara, L.B., 2020. Stress field prediction in cantilevered structures using convolutional neural networks. Journal of Computing and Information Science in Engineering, 20(1). (2019).
26. Ning, Z., Khoubani, A., Evans, T.M., 2015. Shear wave propagation in granular assemblies. Comput. Geotech. 69, 615-626
27. O'Donovan, J., Ibraim, E., O'Sullivan, C., 2016. Micromechanics of seismic wave propagation in granular materials. Granular Matter 18(3), 1-18
28. O'Rourke, M. and Ayala, G., 1993. Pipeline damage due to wave propagation. Journal of Geotechnical Engineering, 119(9), pp.1490-1498.
29. Reddy, J. N. (2006). An Introduction to the Finite Element Method (Third ed.). McGraw-Hill. ISBN 9780071267618.
30. Ronneberger, O., Fischer, P. and Brox, T., 2015, October. U-net: Convolutional networks for biomedical image segmentation. In International Conference on Medical image computing and computer-assisted intervention (pp. 234-241). Springer, Cham.
31. Sbarufatti, C., Manson, G., & Worden, K., 2014. A numerically enhanced machine learning approach to damage diagnosis using a Lamb wave sensing network. Journal of Sound and Vibration, 333(19), 4499–4525. http://doi.org/10.1016/j.jsv.2014.04.059
32. Sorteberg, W.E., Garasto, S., Pouplin, A.S., Cantwell, C.D. and Bharath, A.A., 2018. Approximating the solution to wave propagation using deep neural networks. arXiv preprint arXiv:1812.01609.
33. Takahashi, T., Kondo, T., Saitou, H., Okazaki, T. and Ishikiriyama, M., Toyota Motor Corp, 2000. Method and apparatus for determining gasoline characteristics by using ultrasonic wave. U.S. Patent 6,032,516.
34. Van Pamel A, Brett CR, Huthwaite P, Lowe MJS., 2015. Finite element modelling of elastic wave scattering within a polycrystalline material in two and three dimensions. J. Acoust. Soc. Am. 138, 2326–2336. (doi:10.1121/1.4931445)
35. Van Pamel A, Sha G, Rokhlin SI, Lowe MJS., 2017. Finite-element modelling of elastic wave propagation and scattering within heterogeneous media. Proc. R. Soc. A
36. Zhu, W., Sheng, Y. and Sun, Y., 2017. Wave-dynamics simulation using deep neural networks.