Machine Learning Algorithms for EM Wave Scattering Problems

Anthony James McElwee, *MEng Student, DCU*

Abstract **– This review examines the possibility of using machine learning (ML) algorithms in the search for solutions to Electric Field Volume Integral Equations (VEFIE) formulated, forward scattering problems. A short overview of existing, conventional approaches to approximating solutions to such problems is included, along with a reflection on some recent attempts to augment these methods and create ML emulators by using deep learning (DL) approaches. Based on the review, a brief proposal for the direction of the project activity is offered for deliberation. The aspiration of the review is to communicate recent developments in nascent ML approaches and to provide groundwork for the development of a solver, SolverEMF2, that resolves to reduce the computational cost of providing a solution to the scattering problem at time of inference via a DL model called Prescient2DL.**

Index Terms - computational electromagnetics, deep learning, knowledge integration, neural networks, physics-guided, physics-informed, VEFIE, Volume Electric Field Integral Equation

I. Introduction

A. Task Motivation

The construction of object classifiers using electromagnetic scattering characteristics and the competent planning of wireless network design are undertakings that can require large numbers of frequency-domain simulations and the ability to iteratively adjust input configurations through intervention by a design engineer [1], [2]. Typically, these tasks operate with a constrained set of input parameters, such as incident source and material/geometry attributes of scatters. Although input parameters are comparable across simulation incidences, conventional methods typically require full uninterrupted simulations, below the wavelength, to provide solutions. As a consequence, the generation of large volumes of such simulations takes an uneconomical amount of time and computer memory. Design methodologies appreciate the incorporation of rapidly adjustable, human mediated input configurations but conventional approaches lead to inflexible workflows. In addition, early-stage designs are usually afforded significantly higher error thresholds than full simulations deliver, resulting in over-simulation and a waste of computational resources. With restrictions on the volume of simulations afforded to designers, it is postulated that final classifier metrics and planning layouts are typically sub-optimal.

Just as the requirement to build expensive, physical prototypes in design development workflows has been minimized through the use of computational electromagnetics (CEM), research is now underway to reduce the computationally intense attributes of CEM through the use of data-driven ML. The aim of this project is to accelerate VEFIE-formulated, two-dimensional, scattering simulations at time of inference using ML algorithms in a bid to alleviate the described design workflow issues. The CEM aspect of the problem is acknowledged to have a steep learning curve [3].

Date of submission: 2023/01/22. e-mail: anthony.mcelwee2@mail.dcu.ie

B. Problem Specification

The forward problem constitutes the resolution of scattered wave fields based on information regarding the material contrast and incident field [3]. Typically, Maxwell's equations are formulated in a manner which gives rise to the Helmholtz Wave Equation, which degenerates into Fredholm Integral Equations, through boundary and continuity conditions, in particular, the second kind for VEFIE. The design properties of interest are assumed to depend sinusoidally on time with a shared angular frequency ω.

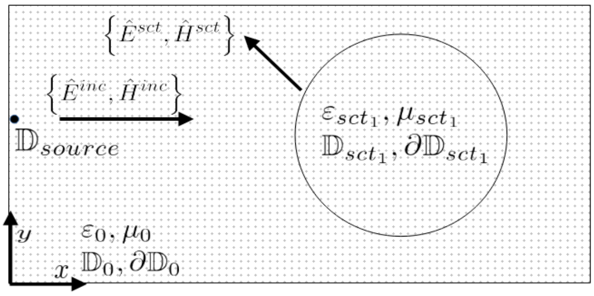

Fig. 1 Problem Illustration. A single source emitting incident waves is located at a fixed x-axis location on the left-hand side of the scatter. Material values are complex valued, frequency-dependent permittivity (ε) and permeability (μ). Background points indicate discretization.

In this project, the aim is to solve for the total electric field $E^{tot}(\boldsymbol{r})$ so that the scattered field, $E^{sct}(\boldsymbol{r})$, can be approximated in the simulation domain, as shown in Fig. 1. Positions in the 2D domain are denoted $\boldsymbol{r} = (x, y)$. A scatterer is located in free-space with surface boundary geometry that will vary in deformation. Material constituents of the scatter give rise to permittivity contrast only, so permeability is assumed to be the same as free-space ($\mu = \mu_0$).

Incident waves, $E^{inc}(\boldsymbol{r})$, are emitted in Transverse Magnetic Mode by a sole transmitter at the left-hand side of the domain. As a result, the incident electric field has no x or y component, only a z one, although Transverse Electric Mode can also be considered with similar consequences.

As given in [1], setting $k_b = \omega\sqrt{\varepsilon_0\mu_0}$ as the wavenumber, the described configuration gives rise to the electric field integral equation:

$$E^{tot}(\boldsymbol{r}) = E^{inc}(\boldsymbol{r}) + k_b^2 \int_D G(\boldsymbol{r} - \boldsymbol{r}')\,\chi(\boldsymbol{r}')E^{tot}(\boldsymbol{r}')d\boldsymbol{r}', r \in D, \quad (\mathbf{1})$$

where $\chi(\boldsymbol{r})$ is the contrast function and $G(\boldsymbol{x})$ is the 2D free space Greens function

$$G(\boldsymbol{r} - \boldsymbol{r}') = -\frac{j}{4} H_0^{(2)}(k_b|\boldsymbol{r} - \boldsymbol{r}'|). \quad (2)$$

It is assumed that no sources exist within scatters. The scattered field, $E^{sca}(r^R)$, can be computed by

$$E^{sca}(r^R) = k_b^2 \int_D G(r^R - \boldsymbol{r}')\,\chi(\boldsymbol{r}')E^{tot}(\boldsymbol{r}')d\boldsymbol{r}', r^R \notin \boldsymbol{D}. \quad (\mathbf{3})$$

A similar formulation in Chapter 3 of [3] is given with more exhaustive derivations for various material assumptions, as well as MATLAB code.

II. Review & Analysis of Prior Work

A. Existing approaches and their related use with ML

Awareness of existing approaches is important when developing SolverEMF2. Concepts underpinning such methods may be assimilated into the DL architecture [4]. Appreciation of computational bottlenecks may also allow Prescient2DL to be specifically targeted.

1) Monte Carlo (MC)

MC methods estimate the value of an integral via repeated random sampling and can evaluate arbitrary points in a domain, including integrals with singularities and discontinuities. The rate of convergence for naïve MC is $\mathcal{O}(\mathrm{n}^{-\frac{1}{2}})$, making it computationally expensive.

2) Analytical

Integrals may admit approximate solution methods, such as infinite series solutions, due to the simple nature of the geometry in the formulation. For VEFIE, these methods are dominated by Bessel-function approaches [3]. Infinite summations can be truncated to suit the required accuracy of the solution, provided the infinite series actually converges analytically. Such solutions are used to benchmark CEM solvers for canonical problems, assess accuracy requirements and debug development code. Analytical methods are also useful for generating initial training data for developing Prescient2DL. When problems contain non-trivial geometries, analytical Bessel-Function approaches breakdown.

3) Conventional Computational Electromagnetics (CEM)

More usually, numerical approximation methods are used for solving VEFIE formulated integrals. They typically use discretized grid systems generating large linear systems of equations [4]. They offer high fidelity solutions for a wide variety of problem formulations, are in widespread use and have been analytically validated for canonical problems [3].

Boundary Element Methods, known idiomatically as Method of Moments (MoM), require the computation of matrix inversions, often using iterative Krylov Methods [3]. It is possible to formulate the integral operator as a discrete convolution and accelerate the matrix inversions by Fast Fourier Transforms [3]. The exploitation of circulant properties of Toeplitz matrices or eigenvalue deflation can also reduce computational requirements. With such formulation adjustments, the rate of convergence for BICGSTAB solver can be reduced to $\mathcal{O}(\mathrm{n}\log n)$ [1].

CEM also covers the Finite Difference Frequency Domain Method (FDFD), Finite Difference Finite Time Method (FDFT) and Finite Element Method (FEM). All CEM require an accuracy threshold or bound on resources as an input so that they can be realized on a computer. As a problem becomes larger, CEM eventually becomes uneconomical in both computational time and memory management [1].

4) High-Frequency and Empirical Approaches

Ray tracing approaches can be used for indoor propagation problems [1]. While the contrary has been reported in [1], ray tracing formulations are typically faster than CEM approaches as they are high-frequency approximations that exploit assumptions from geometrical optics. An example of how developments in ray tracing may stimulate the development of SolverEMF2 is briefly mentioned in the final section of this review. Also considered in [1] are empirical path loss models that may give insight into how DL architectures can be simplified to reduce training burdens.

In summary, existing approaches can be used to generate development data for Prescient2DL, help validate results and offer insights into how SolverEMF2 can be constructed.

B. Possible ML approaches to the problem

In a naïve sense, this a supervised regression problem and deployed ML models can offer an inference in a smaller number of computations than the preferred CEM [5]. A variety of ML algorithms exist and can be appropriated to almost any research domain where data is plentiful. The survey [6] gives a wide overview of application-centric objectives for using ML in engineering and physics domains. With regard to this project, and its resource limitations, exploring downscaling, reduced order modelling, forward PDE solving, inverse modelling, data generation and uncertainty quantification may contribute to development.

One ML development in particular, DL, has led to exceptional advancements in computer vision over the last decade. Indeed, [6] classifies physics-guided methods to integrate scientific knowledge into ML and all are applicable to DL: loss functions; training weight initialization; architecture design; hybrid modelling. Efforts to develop understanding of statistical properties of DL have led to conjectures about the benign nature of its overfitting and how over parameterization leads to tractability when dealing with very complex models. Consequently, DL is now of interest to researchers, more than any other aspect of ML, in trying to combat expensive computational physics problems.

While DL approaches have been more extensively applied to inverse problems, EM scattering forward problems have only recently been reported. Applications of ML to forward problems in other domains can be found more easily. There are research papers reaching back to the 1990s that strive to use neural networks to solve fluid dynamics, process modelling problems and differential equations [7].

C. Surrogate Replacements

Surrogate models, or emulators, are built with the intention of assimilating an entire method, typically CEM, within an approximation model. The surrogate requires minimal human interaction and can be used as a sub-model in a hierarchical framework. The cost of data generation and training is realized in an offline stage prior to deployment time which results in an exchange of computationally intensive algorithms with data-driven inferences. The emulator avoids solving large systems of equations generated by the approximation over basis functions of non-linear integrals, thus removing a computational bottleneck.

As profiled in Chapter 8 of [4], DL architectures have already been proposed as ML duals of CEM methods in a bid to emulate their abstract properties. A variety of Long Short-Term Memory, Convolutional Neural Networks (CNN), Encoder-Decoder structures and Physics-Informed Neural Networks (PINN) are combined with other DL techniques, depending on the approach the CEM captures in its solution.

Surrogates are usually trained for specific problem parameter ranges and, as a result, are assumed to have limited generalization ability [7]. Even with immense advances in ML, these models introduce uncertainties and compromise interpretability and explain-ability of results [7].

Chapter 4.3 of [7] gives a short description of peer-reviewed, non-electromagnetic case studies that used DL surrogates. Typically, training data was constructed from a small number of FEM simulations and used to develop emulators for human tissue stress determination. These surrogates allowed real-time interventions with patients. In further examples, [7] mentions CNN architectures used in field estimation for fluid dynamics. Although accuracy was reduced compared to conventional methods, ML was deemed sufficient for early stage design workflows. In summary of [7], surrogates developed using DL have been deployed to act as decision support mechanisms to humans in medical settings and, in resource restricted design scenarios, emulators enhanced composition methodologies for engineers.

1) Direct solvers using input-output pairs

The paper [8] precedes and forms the groundwork for the new book [9] that reports on the implementation of a U-Net structured emulator. The architecture takes two input images that establish the source as well as the material/geometry of the scatter as depicted in Fig. 2 taken from [8]. In essence, it is an autoencoder styled structure with CNN and residual blocks. The residual blocks help to overcome common problems with training DL networks, via skip layers, and the technique features across the surveyed literature.

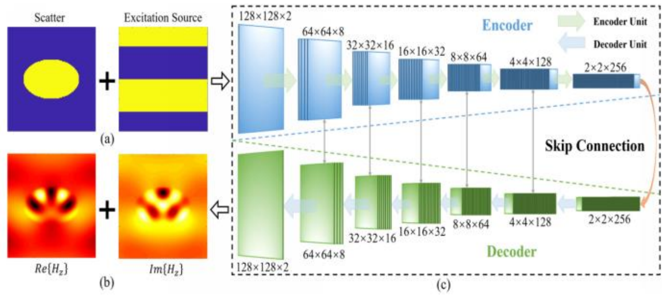

Fig. 2 (a) Input images for scatter & source. (b) Two output images representing Re() and Im() parts of solved field. (c) U-Net Architecture [8].

The problem of estimating complex spatial relationships, where global information influences local values, typically requires deep networks that give rise to vanishing gradients unless the architecture is augmented with said remediation structures.

The paper outlines FDFD discretization for an ellipse and modeling of a TE plane wave is validated against commercial solver COMSOL Multiphysics. The implemented FDFD solver is applied to solve for scattering caused by a 2D training set whose geometry and material properties are coherently bounded by parameter ranges.

One difference between [8] and [9] is that the paper [8] used CReLU activation functions while the book [9] discusses various considered options, finally opting for ELU based on an experiment. Neither of these activation functions are considered immediate choices for DL development. The varied documentation regarding this aspect of the architecture points to the intricacies involved in ML emulator development and that superior DL configurations may yet be found. While [9] uses a mean-squared error loss function to compare the output with the FDFD solution, PINN approaches in the next section offer a different approach to this aspect of the DL training approach.

The test results are presented as having low error when compared to the same FDFD code used to generate training data. In addition, shapes not present in training are evaluated using the emulator and reported error remains low. The paper notes that the emulator does not generalize well for permittivity contrasts beyond the range provided at training. No code was available for either [8], [9]. Explicit experimental documentation is a desirable reproducibility feature when reporting such results.

A more complex surrogate DL architecture, called a General Adversarial Network (GAN), has also been applied to the problem [5]. It uses input-output pairs and reformulates the problem as one of ML image translation. GAN development is currently enjoying success, driven by media attention from beyond the ML community. In [5], the generator is constructed using U-Net architecture, similar to that already described in [8], [9]. Through the addition of a discriminator stage, the approach is redirected to find a solution to a Nash Equilibrium problem. By adding such complexity to the architecture, the discriminator also allows negative examples to be generated and tested. [5] describes in atypical detail the computational complexity of the implementation, as opposed to most literature where such considerations are simplified or ignored totally.

[5] claims improved accuracy over the sole U-Net but also indicates some weaknesses associated with this particular form. GANs typically require multiple adjustments to architectural elements, relative to U-Net, and [5] also adjusts the loss functions in addition to these changes. Much larger training sets are required to compensate for the complex form. The range of contrast permittivity tested is narrow and small in [5] compared to the other literature. It is an open question whether specific EM scattering GANs are the architectures that will yield SOTA results.

2) Physics-Informed Neural Network (PINN)

In [2], a DL model is trained using a Maxwell informed, physics-integrated loss function to find the electric field given scatter geometry and material information, replacing FDFD. The residual is based on the time-harmonic Helmholtz EM Wave Equation. This would be considered a PINN, an area of research that has expanded significantly since 2019. In contrast to [5], [8], [9], where the surrogate is developed using a database of input-output pairs, [2] relies on indirect learning dependent on penalizing the physics-informed loss function. A significant advantage to this approach is that the training process does not require intensive computations to generate the model. In [2], the DL model is coupled with a second stage DL model that helps to solve an inverse optimization design problem.

Where full surrogates are implemented, a solution difference gap relative to CEM is typically not clarified. This uncertainty opens surrogates to questions of robustness. Stating input parameter ranges used in training is frequently the unsatisfactory rebuttal.

D. Combined/Hybrid Methods

As already stated, ML can be used to achieve diverse objectives and knowledge of underlying physics can be infused into DL models in a variety of ways. In the feasibility study [10] regarding DL and the Poisson Equation, the authors give a thoroughly documented demonstration of a CNN based architecture, orientated around Algebraic Multigrid approaches, that can act as a surrogate to solving the PDE or as the provider of an initial guess for a CFD solver to achieve the same aim. The stated aspiration is that the informed guess allows the iterative solver to reach convergence in a smaller *wall-clock* runtime compared to those not given an initial guess. This paper makes an attempt to integrate a variety of approaches mentioned in [6]. [10] gives insights into development, provides narrative around creating special loss functions to enhance training rates and achieve lower error metrics than more typical PINN and MSE loss functions, as well as provide results that include impacts on BICGSTAB initial error rates. An ablation study focuses on changes to model architecture. Although this paper does not examine electromagnetics, it offers fertile ground for development proposals.

While other uses for combined approaches are mentioned in [7], the underlying theme of this hybrid form is that ML acts as a support mechanism for deterministic methods. Many examples exist where ML controlled systems are actively discouraged, such as medical applications. The pervasive attitude is that ML should never be used in a stand-alone fashion but instead aid or accelerate a guided method. Aside from risk aversion, this approach may reduce robustness testing requirements. In the case of supplying initial guesses, this aspect is drastically reduced since deterministic iterative algorithms should converge to a unique solution.

E. Culs-De-Sac

During the review, some pre-print and peer reviewed material presented possible research routes that transpired to be inapplicable or worse. Fundamentally, such material was underpinned by an inappropriate use of DL for directly solving linear problems or through sub-algorithmic augmentation. Their inappropriate nature can be identified from plots of loss and error functions with extreme convergence rates. In these cases, DL adds more computational expense and creates needless uncertainty.

III. Relation of Prior Work to Project Problem

Even though there is a relative poverty of research into the application of ML to forward EM scattering problems, there are already multiple approaches to infusing ML in the construction of new engineering solvers. Acceleration might be achieved by considering new objectives in the engineering workflow, such as increasing design process flexibility. ML may aid in producing early-stage design solvers with small inference times whose estimations are satisfactory for error requirements less stringent than final design criteria.

F. Proposal of the direction of the project activity

The central hypothesis is that ML can be used in a combined-hybrid manner to robustly lower the computational burden of CEM. Based on the cited literature, the project proposes the creation of SolverEMF2 that will encapsulate the entire solution workflow. The computational cost of providing CEM convergent solutions will be reduced via an initial guess, via a DL model called Prescient2DL, to a MoM iterative solver, such as BICGSTAB. SolverEMF2 will then complete the MoM approach with this guess, reducing the iteration count required to achieve convergence.

G. Potential routes of experimentation

Prescient2DL will initially be developed using the existing architectures already cited. Attempting to resolve mathematical features that various CEM methods utilize [4] and synthesizing physics-informed loss functions to reduce required training data and increase robustness [2] are both routes that can be expanded upon. By amending existing architectures, via meta-architectures or assimilating developments in GANs, an EM scattering focused DL architecture may finally diverge from the U-Net architecture originally intended for biomedical segmentation. MATLAB and Tensorflow in Python will be used with Git to facilitate reproducibility.

Finally, light rendering typically also involves solving Fredholm Integral equations of the Second Kind, generally dependent on MC and ray tracing approaches. Significant developments in this domain have occurred recently. Through a multi-staged solver, the challenge of solving VEFIE could be recast as an inverse problem. By iteratively populating MC samples in the forward manner, a DL model in the second stage could denoise the inferred field as SolverEMF2 converges to the MoM validated solution. This approach may be less resource intensive than developing GAN structures.

IV. Conclusion

The sources considered in the process of completing this literature review agree on the positive potential of ML to shift the computational effort of current conventional approaches from time of inference to the training stage, as well as reduce the required duration to provide a solution to the problem of electromagnetic scattering. The review finds DL as the best route that presents experimental opportunities.

References

[1] I. Kavanagh and C. Brennan, 'Validation of a volume integral equation method for indoor propagation modelling', *IET Microwaves, Antennas & Propagation*, vol. 13, no. 6, pp. 705–713, 2019, doi: 10.1049/iet-map.2018.5849.

[2] J. Lim and D. Psaltis, 'MaxwellNet: Physics-driven deep neural network training based on Maxwell's equations', *APL Photonics*, vol. 7, no. 1, p. 011301, Jan. 2022, doi: 10.1063/5.0071616.

[3] P. M. van den Berg, *Forward and inverse scattering algorithms based on contrast source integral equations*. Hoboken, NJ: Wiley, 2020. [Online]. Available: https://onlinelibrary.wiley.com/doi/book/10.1002/9781119741602

[4] M. Martínez-Ramón, A. Gupta, J. L. Rojo-Álvarez, and C. G. Christodoulou, *Machine learning applications in electromagnetics and antenna array processing*. Boston London: Artech House, 2021.

[5] Z. Ma, K. Xu, R. Song, C.-F. Wang, and X. Chen, 'Learning-Based Fast Electromagnetic Scattering Solver Through Generative Adversarial Network', *IEEE Transactions on Antennas and Propagation*, vol. 69, no. 4, pp. 2194–2208, Apr. 2021, doi: 10.1109/TAP.2020.3026447.

[6] J. Willard, X. Jia, S. Xu, M. Steinbach, and V. Kumar, 'Integrating Scientific Knowledge with Machine Learning for Engineering and Environmental Systems', *ACM Comput. Surv.*, vol. 55, no. 4, pp. 1–37, May 2023, doi: 10.1145/3514228.

[7] S. Kollmannsberger, D. D'Angella, M. Jokeit, and L. Herrmann, *Deep Learning in Computational Mechanics: an Introductory Course*. Cham: Springer, 2021.

[8] S. Qi, Y. Wang, Y. Li, X. Wu, Q. Ren, and Y. Ren, 'Two-Dimensional Electromagnetic Solver Based on Deep Learning Technique', *IEEE Journal on Multiscale and Multiphysics Computational Techniques*, vol. 5, pp. 83–88, 2020, doi: 10.1109/JMMCT.2020.2995811.

[9] Q. Ren, Y. Wang, Y. Li, and S. Qi, *Sophisticated Electromagnetic Forward Scattering Solver via Deep Learning*. Singapore: Springer, 2022. doi: 10.1007/978-981-16-6261-4.

[10] A. G. Özbay, A. Hamzehloo, S. Laizet, P. Tzirakis, G. Rizos, and B. Schuller, 'Poisson CNN: Convolutional neural networks for the solution of the Poisson equation on a Cartesian mesh', *DCE*, vol. 2, p. e6, 2021, doi: 10.1017/dce.2021.7.