

School of Electronic Engineering

CB54: Machine Learning Algorithms for EM Wave Scattering Problems

Portfolio

Anthony James McElwee ID Number: 20211330

August 2023

MEng in Electronic and Computer Engineering
Supervised by Dr Conor Brennan

Declaration

I hereby declare that, except where otherwise indicated, this document is entirely my own work and has not been submitted in whole or in part to any other university.

Signed: Live Date: 2023/08/20



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Conference Paper

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Machine Learning Algorithms for EM Wave Scattering Problems

Anthony James McElwee, MEng Student, DCU

Abstract – This is the abstract. Index Terms – index term 1

I. INTRODUCTION

A. Task Motivation

The task motivation.

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The problem specification. [1]

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This is the conclusion.

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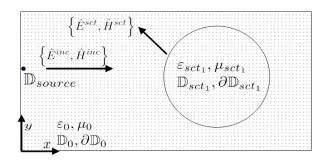


Fig. 1 Problem Illustration. A single source emitting incident waves is located at a fixed x-axis location on the left-hand side of the scatter. Material values are complex valued, frequency-dependent permittivity (ϵ) and permeability (μ). Background points indicate discretization.

 $Date\ of\ submission:\ 2023/08/21.\ e-mail:\ anthony.mcelwee 2@\ mail.dcu.ie$



School of Electronic Engineering

CB54: Machine Learning Algorithms for EM Wave Scattering Problems

Literature Survey

Anthony James McElwee ID Number: 20211330

January 2023

MEng in Electronic and Computer Engineering
Supervised by Dr Conor Brennan

Declaration

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Signed: Authory Tunes MC Elwee

Date: 2023/01/23

Machine Learning Algorithms for EM Wave Scattering Problems: Literature Review

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, physicsinformed, 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].

 $Date\ of\ submission:\ 2023/01/22.\ e-mail:\ anthony.mcelwee 2@\ mail.dcu.ie$

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 .

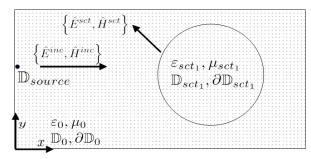


Fig. 1 Problem Illustration. A single source emitting incident waves is located at a fixed x-axis location on the left-hand side of the scatter. Material values are complex valued, frequency-dependent permittivity (ϵ) and permeability (μ). Background points indicate discretization.

In this project, the aim is to solve for the total electric field $E^{tot}(\mathbf{r})$ so that the scattered field, $E^{sct}(\mathbf{r})$, can be approximated in the simulation domain, as shown in Fig. 1. Positions in the 2D domain are denoted $\mathbf{r}=(x,y)$. 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, $E^{inc}(\mathbf{r})$, 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:

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

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

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

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

$$E^{sca}(r^R) = k_b^2 \int_D G(r^R - \boldsymbol{r}') \, \chi(\boldsymbol{r}') E^{tot}(\boldsymbol{r}') d\boldsymbol{r}', r^R \notin \boldsymbol{D}.$$
 (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 $\mathcal{O}(n^{-\frac{1}{2}})$, 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 $\mathcal{O}(n \log n)$ [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.

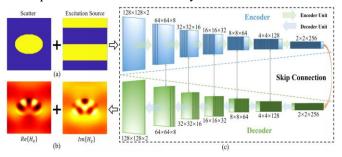


Fig. 2 (a) Input images for scatter & source. (b) Two output images representing Re() and Im() parts of solved field. (c) U-Net Architecture [8].

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.

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Project Design Plan

Anthony James McElwee

ID Number: 20211330

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Project Design Plan

Research Question

The student proposes to sub-divide the research question into two stages to allow for iterative assessment of plausibility of research opportunities and increased agility around the resource and time constraints available.

- The primary stage is aimed at establishing elements of the work of [1]–[5] in a reproducible workflow called SolverEMF2 and creating a supervised regression model called Prescient2DL to test the various hypothesis associated with the Primary Research Question, as explained in the Design Approach section.
- The secondary stage is based around investigating the rudiments of Prescient2DL. Possible aspects for analysis are covered in the various hypothesis associated with the Secondary Research Questions, as explained in the Design Approach section.

Primary Research Question

"Can the manner in which deep learning has been shown to solve two-dimensional, forward electromagnetic scattering problems applied to the problem of predicting EM wave propagation over rural terrain be improved upon?"

As already reported in the Literature Review, various sources have described using deep learning to tackle forward electromagnetic scattering problems, however, to the knowledge of the student, none have provided a public, reproducible, open-source workflow or a model to the research community. The student proposes to approach the integration of the developed deep learning model, Prescient2DL, into SolverEMF2 through the use of Prescient2DL to generate initial guesses for the Krylov Iterative Solver. By establishing the SolverEMF2 workflow, this primary research question will be approached through the investigation of simulations with several segmented statistical hypothesis tests in lieu of qualitive mathematical proofs. Implicitly, the primary aim of the project is to implement a solver with a deep learning model that optimally shifts calculation metrics to towards the lower left corner of the Residual Error versus Iterations/Time graph when solving permittivity contrast source only Volume Electric Field Integral Equations.

Secondary Research Questions

The secondary research questions below are based around trying to expand knowledge around whether the application of deep learning to this domain is fundamentally underpinned by the attributes of the training data set or whether a hierarchical approach to model generation exists. The questions offer a rich range of potentially publishable findings and opportunities to contribute to the field of scientific machine learning.

"Are all models equal in the framework of the performance analysis conducted in the primary research question? Can improvements be made to model development approaches? Can model deployment be improved so that there is an increased opportunity/impact by the model on SolverEMF2 performance?"

Based on the literature review, and echoed in the more recent [6], the models reported in the available literature are either developed in a U-net based architecture or through a Physics Informed Neural Network (PINN). The student proposes to conduct studies into the performance between siloed models to illustrate advantages and changes in performance given a consistent testing environment.

From the insights arising from the model comparison stage, the student believes that these approaches can initially be expanded upon and ensembled. Stemming from this investigation will be the final Prescient2DL model that should demonstrate a more mature application of deep learning to the problem domain. This facilitates the exploration of deep learning attributes and features specifically refined for the problem domain with the possibility of reporting on refined architectures or properties of the model development purpose previously not recorded in journals.

As reflected in the literature review, there is almost no diversity in the deployment strategies for deep learning in this problem domain. The process of emulation is the baseline approach to harnessing deep learning

models. The model is expected to resolve problems whose inputs are confined to the parameter ranges associated with the input data used to train the model in the first place. The online-stage of the process thus mirrors the use of Look-Up Tables (LUTs) in conventional problem approaches. The primary stage aims to expand this baseline approach by wrapping Prescient2DL solutions in the Method of Moments framework. In addition to this expansion, the literature review has highlighted sub-algorithmic adjustments to Krylov Iterative Solvers that may yield improved performance metrics. The area of probabilistic numerics may also offer alternative ways that deep learning can be integrated into SolverEMF2.

The benchmarking and characterisation of existing model formulations, the expansion of the model development approaches and the deployment techniques used in SolverEMF2 should facilitate investigation into the generalisability of the deep learning in the domain. The use of Prescient2DL as a basis for transfer learning may also be investigated. These secondary research questions will also be approached through the investigation of several segmented statistical hypothesis tests in lieu of qualitive mathematical proofs.

Project Scope

- The electromagnetic formulation that underpins the area will remain as the two-dimensional, permittivity contrast source only Volume Electric Field Integral Equation as derived at equation (6.5) in [2] or equation (3.86) in [3]. These are scalar integral equations. The derivations in [2] and [3] differ in their uses of time harmonic convention, however, the results from the equations should be equivalent. The Time Harmonic Dependence Convention (j=-i) can be used to translate between them. In [2], the Real-Value Transform with complex notation "i" is used while in [3] the Laplace Transform with complex notation "j" is favoured with the Laplace variable $s=-i\omega$.
- Establish a fresh Github version control repository for code maintenance and sharing.
- Develop the initial SolverEMF2 by migrating VEFIE code from MATLAB to Python and validating the code on a canonical problem. The student has purchased a new laptop with i7-11800H @ 2.3GHz CPU and NVIDIA GeForce RTX 3070 GPU. Access has also been granted to remote DCU GPU rigs and these will be utilised as the project matures.
- Establish and follow the dataset generation pathway as outlined in the Design Approach section below.
- Develop the initial iteration of Prescient2DL using Python deep learning packages.
- There are a number of advanced research areas outlined in the Literature Review, such as the expansion of models via Monte Carlo integration. Due to resource/time constraints, the student proposes to only approach these areas if the potential of the research questions, as outlined in the previous sections, has been exhausted.
- The visualisation and flexibility of the solution information conveyed to the user of SolverEMF2 was initially of much interest to the student, however, since the literature review was conducted the student has discovered a project hosted at (https://github.com/chiuhans111/fdtd-html). That project tackles a timedomain, rather than frequency-domain, problem but the student proposes to focus on the more technical performance metrics and deep learning model development due to the increased probability of generating publishable content.

Design Approach

Code Development Environment

Code will be developed in a manner where all outputs are reproducible through input documentation and seeding. Metrics around the non-DL simulations will be recorded. Time of training and time of inference with initial error (for hybrid models incorporated into conventional methods) will also be recorded.

Code Development Validation – Initial MATLAB migration

Verify code through the solution of canonical toy problems in MATLAB and Python, comparing results to a satisfactory degree of accuracy.

Deep Learning Dataset Development-Pathway

The creation of a benchmark dataset would be a publishable accomplishment in itself. The student proposes to start with a simple, narrow parameter settings database and as the feasibility of a model develops, the student plans on adding network architecture complexity.

- In the first instance, only train the model on data generated from canonical problem formulations with Bessel-function type solutions. Then benchmark an independent conventional model (MoM) against the Bessel-Function solutions and the ML model. If all three agree then the ML model can be trained next on the conventional model.
- Generate non-canonical dataset using MoM python code.
- Generating the training dataset will be computationally intensive. The student proposes to squeeze value
 out of the simulations by using data augmentation such as rotation and reflection. A large number of
 simulations should be possible by having a range over the input parameters.

SolverEMF2 - Architecture

The architecture of SolverEMF2 initially sets all guesses to the Krylov Iterative Solver as an array of zeros. This step is later replaced with Prescient2DL informed guesses. The student proposes following the development of the solver methodology using the pathway illustrated in the image below. The student does not anticipate that the later Monte Carlo stages will be achieved in the time limitations of the project.

SolverEMF2 Solution Approaches

Updating Monte Carlo Simulator with DL Denoiser Model

Relative Effort: High

Features: Iteratively update with Monte Carlo samples and then use a DL denoiser model to solve.

Computational Complexity: Unknown, wrapping this in Biconjugate Gradient Stabilized Method is a further option.

Flexibility: Medium as dependent on ability to view Monte Carlo updates.

DL Emulator LUT as Initial Guess for Biconjugate Gradient Stabilized Method with Monte Carlo updating.

Relative Effort: High

Features: Convergence check at deployment. Iteratively update domain regions that are computationally important with Monte Carlo samples, especially regions that are far from source where scattering effects are largest.

Computational Complexity: Depends on iterative convergence but addition of Monte Carlo may be a trade-off.

Flexibility: Medium as dependent on ability to view Monte Carlo updates and examine iterative stage intermediate results.

DL Emulator LUT as Initial Guess for Biconjugate Gradient Stabilized Method

Relative Effort: Medium

Features: Convergence check at deployment.

Computational Complexity: Depends on DL model architecture in addition to a lower bound of one iteration of iterative method to achieve convergence. Flexibility: Low as dependent on ability to examine iterative stage intermediate results.

DL Emulator LUT (Total Replacement)

Relative Effort: Lowest

Features: No convergence check at deployment; totally dependent on training stage experimental validation.

Computational Complexity: Depends on DL model architecture.

Flexibility: None as only a single pass is completed.

Prescient2DL - Architecture

The student proposes to follow the pathway outlined in the image below when expanding the model architecture and physics infusion.

Prescient2DL Architectural Development

GANs / Archtech House Ideas / Denoiser

DENSE Meta-architecture search & sub-algorithmic infusion

PINNs / MawellNet Regularisation

U-Net

Primary Research Test 01 – Initial Solution Conveyance t-Test

Null Hypothesis H₀: The initial error (Residual Norm) in the Krylov Iterative Metrics in SolverEMF2 is the same as for the non-DL assisted conventional solver.

Alternative Hypothesis H_A : The initial error (Residual Norm) in the Krylov Iterative Metrics in SolverEMF2 is lower than the non-DL assisted conventional solver.

Note: Conveyance is used to mean an indication of the level of information from the informative guess, be it Prescient2DL or a more vanilla approach, conveyed to SolverEMF2. The closer the Kyrlov Iterative Solver is to the be within the acceptable solution threshold, with respect to the naïve guess, then the more useful information has been conveyed via the guess. In the Test 01 situation, this manifests as simply the lower initial error.

Primary Research Test 02 - Solution Convergence t-Test

Null Hypothesis H₀: A linear approximation of the slope of the curve for plot Residual Norm versus Iteration Count, labelled as convergence rate, in the Krylov Iterative Metrics for SolverEMF2 is the same as for the non-DL assisted conventional solver.

Alternative Hypothesis H_A: A linear approximation of the slope of the curve for plot Residual Norm versus Iteration Count, labelled as convergence rate, in the Krylov Iterative Metrics for SolverEMF2 is the not equal to the non-DL assisted conventional solver.

Note: Further tests to establish if the absolute value of the slope is greater for Solver EMF2 may be required, however, it is expected that the convergence rate will remain unless sub-algorithmic integration of the model is successful in the secondary stage.

Primary Research Test 03 – Solution Conveyance t-Test

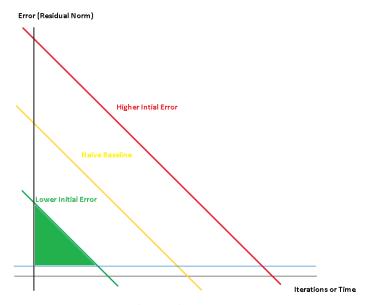
Null Hypothesis H₀: The area under the curve for plot Residual Norm versus Iteration Count, labelled as AbsementKIM, in the Krylov Iterative Metrics for SolverEMF2 is the same as for the non-DL assisted conventional solver.

Alternative Hypothesis H_A: The area under the curve for plot Residual Norm versus Iteration Count, labelled as AbsementKIM, in the Krylov Iterative Metrics for SolverEMF2 is smaller than for the non-DL assisted conventional solver.

Explanation: If both the Residual Norm and the Iteration/time vary, it may be difficult to judge the difference in performance based on a single parameter. This naïve approach to combining the parameters by finding the area under the curve intersecting the two axis may be a way to compare the computational expense expended by the various SolverEMF2 variants. AbsementKIM stands for Absement Krylov Iterative Method and is analogous to Absement in the domain of kinematics.

Secondary Research Tests – General

All tests conducted in the Primary Research Test stage will be applied to the secondary stage. To illustrate the idea of the primary metric from the Primary Research Test, the diagram below shows the baseline permutations that could arising when comparing the output metrics of the SolverEMF2 activities. The diagram on the left indicates an impact on initial errors while the right diagram indicates an impact on the rate of convergence of the solver. Both of these changes of parameter could change simultaneously so a third graph showing the exhaustive list of such graphs could be produced but is deemed too busy to be informative. The areas in green indicate the AbsementKIM that may arise. A smaller AbsementKIM in the final metrics would indicate that more information in general was passed through the initial guess relative to whatever configuration that was used to establish the null.





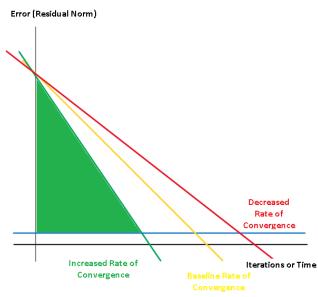


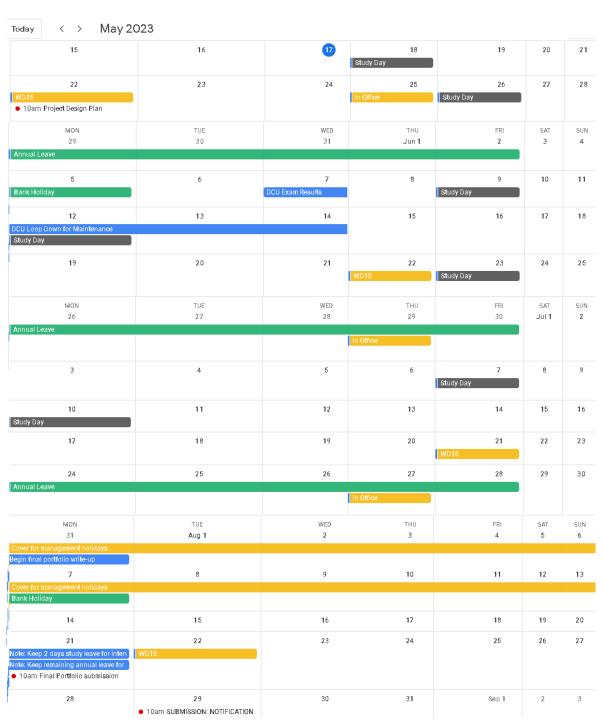
Figure 2: Impacts on Rate of Convergence. Initial error is held constant

Secondary Research Tests - Model Development & Integration

The metrics used in the development process for Prescient2DL will be the residual sum of squares normally used in such regression problems. The developments will follow the baseline established in [1], [4] and expand to include aspects highlighted in the Literature Review. The generalisability of the model will be tested by generating a random shapes dataset, as opposed to the terrain dataset used in the rest of the project. Machine learning models are largely data-driven but the data in this experiment will be totally synthetic. As a result, the developed ML model will be derived from governing equations that are an idealization and representative of that centric world-view. This is the same idea as the Helio-centric versus Geo-centric interpretation in inter-planetary motion. The objective is to build an ML model of an existing conventional method. Testing generalizability could be done by seeing how far Prescient2DL diverges from canonical solutions when initially only trained on canonical datasets, then trained on general datasets, then compare the model on canonical validation set and general test set to see if performance degrades on the canonical test in order to generalize to the generalized inputs. A decision around metrics may also be required, for example, tolerance of some extra resources for time of inference may be tolerated for lower error and vice-versa.

Timeline

As of the date of the submission of this project proposal document (2023/05/21) there are only 92 days to the final submission deadline for the completed project (2023/08/21). In this period, there are 64 weekdays and 28 weekend days. The student has 7 study leave days and up to 23 annual leave days from work. Due to the constraints of work, it is highly likely that not all of the annual leave can be taken in this period. In August, the student will be required to act as cover for management. There is also a strong bias towards taking leave towards the end of the month to avoid impact on the bulk of regulatory reporting between working days 8 and 15. The student is populating the Google Calendar facility, available with their DCU email account, with key milestones and constraints. This is illustrated below. Due to the iterative and unknown time requirements for the tasks outlined in the Project Scope and Design Plan, the student has avoided pinning dates to specific actions with the exception of "Final Portfolio Write-Up". Due to severe constraints in August, the preparation for the final portfolio will need to commence at the start of August and while experimentation can run in parallel in the background, it is highly unlikely that new developments or additions to the model development architecture will be completed beyond this date.



Success Criteria

The student proposes that the criteria for success remain open-ended with the aspiration of completing all items on the list below while acknowledging that the time and resource constraints may curtail its completion. Chapter 13 of [6] offers some open problems in the domain of applying DL to electromagnetic problems. The relevant ones for this specific subdomain can be summarised as trying to generate more generalisable models using less data in a more efficient manner without overfitting. The suggestion is to enhance the model architecture with physically-based loss functions and generate foundation-type models that can be adapted and fine-tuned via transfer learning approaches.

- Validated literature review. See log entry relevant to [6].
- 10 research log submissions updating work progress and developments in the field.
- Python implemented SolverEMF2 workflow that can be used and expanded in future by students of the field.
- Mature Prescient2DL model architecture that can be deployed to accelerate the generation of solutions to these types of problems.
- A dataset of solved simulations for future use by researchers in this field.
- A completed final report portfolio for submission to DCU for masters accreditation that provides answers to the outlined primary and secondary research questions.
- A paper on (https://arxiv.org/) or in a peer-reviewed journal reporting some finding from the second stage of research questions.

Bibliography

- [1] C. Brennan and K. McGuinness, "Site-specific Deep Learning Path Loss Models based on the Method of Moments." arXiv, Feb. 02, 2023. doi: 10.48550/arXiv.2302.01052.
- [2] V. Pham-Xuan, "Accelerated iterative solvers for the solution of electromagnetic scattering and wave propagation propagation problems," doctoral, Dublin City University. School of Electronic Engineering, 2016. Accessed: Mar. 20, 2023. [Online]. Available: https://doras.dcu.ie/20951/
- [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] 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.
- [5] 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.

Lowe Brenner

[6] A. P. M. Li, M. Li, and M. Salucci, *Applications of Deep Learning in Electromagnetics: Teaching Maxwell's Equations to Machines*. Institution of Engineering & Technology, 2023.

Approval

Signature of Project Worker:

Date: 2023/05/20

Print name of Project Worker: **ANTHONY JAMES MC ELWEE**

Signature of Project Supervisor:

Date: 2023/05/21

Print name of Project Supervisor: DR CONOR BRENNAN



School of Electronic Engineering

CB54: Machine Learning Algorithms for EM Wave Scattering Problems

Project Research Log

Anthony James McElwee

ID Number: 20211330

August 2023

MEng in Electronic and Computer Engineering

Supervised by Dr Conor Brennan

Please read before making entries in this log

The purpose of this Project Research Log is to capture concise, focused summaries of research materials you read, as you progress through your project. The emphasis is to record (i) how the material you have read will determine or influence your project solution approach and (ii) your assessment of the key strengths and weaknesses of the solutions, methods, technologies, etc. proposed in the material you have read.

In the first stage of your project, the literature review, use the Log to capture this information for the key papers you have read (for example, the three most important papers of your 10 literature review references). As your project progresses into the design and implementation phases, you will need to continue to search the literature so you can review, revise and refine your initial thinking and the details of your approach to a project solution. Use this Research Log to capture your continued research reading and its influence on your project design and implementation. Be selective about what you record in this log. Do not use it as an informal notebook while you are reading a new paper. Only make an entry after you have read a paper that you consider important to the development of your project solution. It is expected that, by the end of the project, you will have made between 10 and 20 entries (20 maximum). Share your log with your supervisor for viewing throughout the project. You will submit the final version of the log for grading, at the end of the project implementation period. It will be assessed on the basis of how well you have used your analysis of the literature to inform your project design, implementation and the evaluation of your project results. The Research Log contributes 5% to the overall project mark.

Note: All entries you make in this log must use the prescribed format shown on the next page. You will maintain other notes as you progress through your project but they should not be recorded here. Fill in the details where the *** signs are.

Contents

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Log Entry 00: 2022/11/28

Statement of project problem / research question (maximum 200 words)

This statement should be periodically reviewed and updated, as necessary, as your project progresses and you gain further insight into the detailed project challenges, requirements and objectives as your project work moves from background reading, literature review, initial project design planning and detailed design and implementation. Initially, start by stating your current understanding of the project objectives. After each meeting with your supervisor, review and refine your project problem statement, as required.

THIS IS JUST TO RECORD THE INITIAL PROJECT STARTING POINT

"When an electromagnetic wave encounters an object it scatters, with some energy being transmitted into the object and the rest propagating in a variety of directions depending on the material composition and local geometry. A precise knowledge of the scattering phenomenon is desirable for a variety of applications, such as medical imaging, radar and wireless communications. Numerical techniques such as the method of moments give highly accurate results, but are computationally expensive. An emerging alternative is the use of machine learning tools that can be trained using a training set of data covering a sufficiently wide feature set (i.e. problem geometry, material, frequency etc). This project will use an in-house, Matlab-based, implementation of the method of moments to train an artificial neural network to solve the problem of EM scattering from convex dielectric bodies."

A complete reference for the paper

Summary of paper (maximum 100 words)

How is this paper relevant to solving your project problem or addressing your research question? (maximum 100 words)

What are the strengths and weaknesses of the solutions/methods/technologies proposed in this paper? (maximum 100 words)

Log Entry 01: 2023/05/16

Statement of project problem / research question (maximum 200 words)

"Can the manner in which deep learning has been shown to solve two-dimensional, forward electromagnetic scatting problems applied to the problem of predicting EM wave propagation over rural terrain, namely emulation, be expanded or improved upon?"

As already reported in the Literature Review, various sources have described using deep learning to tackle forward electromagnetic scattering problems, however, to the knowledge of the student, none have provided a public, reproducible, open-source workflow or a model to the research community. The student proposes to approach the integration of the developed deep learning model, Prescient2DL, into SolverEMF2 through the use of Prescient2DL to generate initial guesses for the Krylov Iterative Solver. By establishing the SolverEMF2 workflow, this primary research question will be approached through the investigation of simulations with several segmented statistical hypothesis tests in lieu of qualitive mathematical proofs. Implicitly, the primary aim of the project is to implement a solver with a deep learning model that optimally shifts calculation metrics to towards the lower left corner of the Residual Error versus Iterations/Time graph when solving permittivity contrast source only Volume Electric Field Integral Equations.

A complete reference for the paper

[1]

[1] A. P. M. Li, M. Li, and M. Salucci, *Applications of Deep Learning in Electromagnetics: Teaching Maxwell's Equations to Machines*. Institution of Engineering & Technology, 2023.

Summary of paper (maximum 100 words)

This is a new book (2022) dealing with the application of deep learning to electromagnetic problems that the student did not know existed until 2023/05/08 well after the literature review was submitted. The student has read the relevant chapters 1, 2 and 13 of this book and it conforms with the student's literature review with strong overlaps in the references covered. The student views this an as independent confirmation that their research to date and literature review reflects much of the current research energy in the project domain.

How is this paper relevant to solving your project problem or addressing your research question? (maximum 100 words)

In Chapter 13 there is a section dealing with the pros and cons of using DL in the domain whose synthesis would be helpful in the final project portfolio.

Chapter 13 also raises some problems that may be faced in the project. There is a lack of transparency and understanding of the inner workings of the DL architectures. The student believes there are developments in ML space that are working on reducing this lack of transparency, for example, Professor Paul Whelan's visualization methodology for the various layers in the Computer Vision module assignment and the student's understanding that a recent new research domain of explainability in DL may have yielded recent breakthroughs.

What are the strengths and weaknesses of the solutions/methods/technologies proposed in this paper? (maximum 100 words)

One difference to the literature review was that there seems to be a greater consideration given to the subalgorithmic approaches (references 126-130) that the student had partially avoided. As a result the student may reconsider these approaches and consider their inclusion. The sources not previously considered in the literature review have been recorded in the student's Zotero database for future consideration. In terms of downsides of the book, there was nothing that the student hadn't previously considered or covered in the literature review already.

Log Entry 01: 2023/06/01

Statement of project problem / research question (maximum 200 words)

"Can the manner in which deep learning has been shown to solve two-dimensional, forward electromagnetic scatting problems applied to the problem of predicting EM wave propagation over rural terrain, namely emulation, be expanded or improved upon?"

A complete reference for the paper

[1]

[1] A. P. M. Li, M. Li, and M. Salucci, *Applications of Deep Learning in Electromagnetics: Teaching Maxwell's Equations to Machines*. Institution of Engineering & Technology, 2023.

Summary of paper (maximum 100 words)

How is this paper relevant to solving your project problem or addressing your research question? (maximum 100 words)

What are the strengths and weaknesses of the solutions/methods/technologies proposed in this paper? (maximum 100 words)

Log Entry 02: 2023/MM/DD

Statement of project problem / research question (maximum 200 words)

"Can the manner in which deep learning has been shown to solve two-dimensional, forward electromagnetic scatting problems applied to the problem of predicting EM wave propagation over rural terrain, namely emulation, be expanded or improved upon?"

A complete reference for the paper

[1]

[1] A. P. M. Li, M. Li, and M. Salucci, *Applications of Deep Learning in Electromagnetics: Teaching Maxwell's Equations to Machines*. Institution of Engineering & Technology, 2023.

Summary of paper (maximum 100 words)

How is this paper relevant to solving your project problem or addressing your research question? (maximum 100 words)

What are the strengths and weaknesses of the solutions/methods/technologies proposed in this paper? (maximum 100 words)

Complete Bibliography

[1] A. P. M. Li, M. Li, and M. Salucci, *Applications of Deep Learning in Electromagnetics: Teaching Maxwell's Equations to Machines*. Institution of Engineering & Technology, 2023.



Risk Assessment Experimental Method Form for Undergraduate and Taught PG Projects

All operations/procedures being assessed (give specific details):

All operations/procedures are purely theoretical or computational requiring no written risk assessment.

An operations/procedures are purery theoretical of computational requiring	g no written risk assessment.
Risk Category Rating:	
E	
Known or expected hazards associated with the activity:	
None	
Precautions to be taken to reduce the level of risk:	
None	
Training prerequisite:	
None	
Risk remaining:	
None	
Emergency procedures:	
None	
Detail references if any:	
For the Project Worker and Project Supervisor:	
We have carried out a risk assessment for the above operation/procedure	in accordance with those guidelines as detailed in th
School Safety Handbook.	
Signature of Project Worker:	Date: 2023/02/05
Print name of Project Worker: ANTHONY JAMES MC ELWEE	
Lowa Brenner	
Signature of Project Supervisor:	Date 27/02/2023
Print name of Project Supervisor: DR CONOR BRENNAN	

Print name of Technical Officer assigned to Project: CONOR MURPHY

N.B.

- Copies of completed forms should be submitted to the Project Supervisor and the Technical Officer assigned to the project.
- A signed copy of the completed form should be kept in close proximity to the project bench/space where the project is taking place.