IN-SENSOR THIN-FILM MAGNETICS WITH RESERVOIR COMPUTING

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Contents

1 Introduction

This project is a study into the feasibility of biosensors comprised of thin magnetic films acting as reservoirs in the context of Reservoir Computing, a novel machine learning technique that embeds neural computation in the natural properties of a physical substrate. A single output layer of neurons is trained to read changes in one or more fundamental states of the reservoir, and extrapolate the causal input to the physical medium. Thin-films are grown epitaxially and structures can be assembled with nanoscale dimensions, featuring clear magnetic properties. A vast number of biological mechanisms take advantage of ionised elements and their movement. These particles generate fluctuating magnetic fields and it is hoped that these are of sufficient intensity to measurably change the polarisation of a magnetic nanostructure, such that the output layer of neurons can learn to infer patterns that may equate to events in the associated biology. This project aims to assess feasibility in each of the umbrella concepts that govern this implementation, such that the degree of remuneration from continuing this line of exploration is unequivocal. Due to the inherent difficulties and extreme costs associated with manufacturing one-off nanostructures, all physical elements will be simulated in software, with the University of York's in-house atomistic simulator: Vampire. Furthermore, in light of the strengths, scalability and flexibility of high level programming languages, the neuron output layer will be emulated in Python. Developing the moving parts of the project in software increases portability and format compatibility between shared datasets. See section 3 for a breakdown of the project's main academic categories, whereas suggested implementations can be found in section 4.

2 Software Requirements

Software	**Purpose**
VAMPIRE 6	Simulate thin magnetic film structures.
PYTHON3: PyCharm	Emulate and train output layer of reservoir computer.
RASMOL/POV-RAY	Visualise output files of Vampire simulations.
LINUX OS	Vampire & Python.
MICROSOFT OFFICE	View, store, represent data.
LATEX OVERLEAF	Report writing.

3 Literature Review

3.1 Reservoir Computing

Life cannot be paused, it is a vital perpetuation of complex chemistry in time. This percolates down to all constituent mechanisms in biology, dynamic chemical soups in constant, ordered, flux. The study of biological phenomena is invariably time-dependant and any machine learning technique devised to analyse any such dataset needs to accurately capture state-evolution through time. For use in a biosensor context, the network has to be capable of real-time computation on temporal inputs. Feed forward networks have been demonstrated capable of temporal analysis, yet this has repeatedly proven exceptionally difficult and computationally expensive [1]. Liquid State Machines (LSM) were proposed by Maas as a novel Recurring Neural Network (RNN) architecture that could excel at real-time computation [2]. There are specific properties that LSMs must possess in order to guarantee real-time computation on temporal inputs. In terms of topology, the network must be comprised of a randomly connected filter stage with fixed weights, that projects onto a trainable perceptron layer. The filter must be constructed so that it possesses the point-wise separation property. This is tantamount to having a fading memory, such that the distance in time between trajectories of internal states is roughly proportional to the delay between input streams that caused them [3]. In Reservoir Computing (RC) literature, which unifies LSMs and the closely related Echo State Network (ESN) in one field [4], this is referred to as the Echo State Property (ESP) [5]. Furthermore, the readout must possess the universal approximation property, which can be shown is satisfied by a linear regression function [6]. The most commonly used learning algorithm in RC is Ridge Regression, desirable for its simplicity and efficacy in offline scenarios, which couples perfectly with a priori datasets. The biosensor proposed in this project would undergo the training stages in the factory prior to being implanted, hence the focus on previously extruded datasets despite the end-goal being a real-time detection system. The high-dimensionality of the filter stage - the reservoir - introduces enough complexity that a simple linear readout can capture transient information from the input stream. Due to the architecture's highly desirable marriage of simplicity and efficacy, researchers have already explored its capabilities in high accuracy sensor assemblies, with very positive results [7, 8]. There are no requirements in RC for the reservoir to be a neuron-based system, so long as the ESP is preserved. This naturally lead some to investigate the feasibility of using a physical substrate with non-linear dynamics and fading memory instead of a traditional RNN, with surprising success. In a brilliant tour de

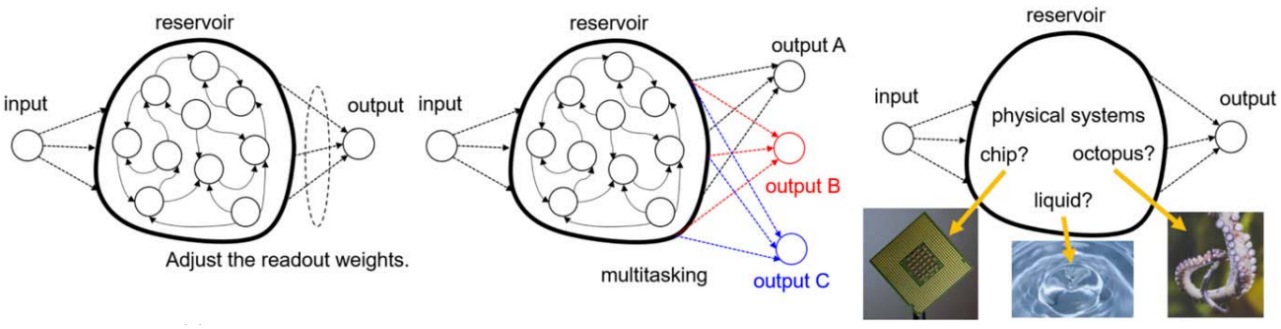

Figure 1: Example of RC architecture. The reservoir is a black-box dynamical system with random connectivity. The broad definitions of what can constitute a reservoir imply that any physical substrate with sufficient non-linear complexity and fading memory is permissible within the framework. Image sourced from [9].

force, Fernando and Sojakka proved that a bucket of water could be utilised to capture complex dynamics in real-time, capable of solving the XOR benchmark problem [3]. See Figure 1 for a conceptualisation of the RC paradigm.

A whole host of physical mediums have been proposed as suitable candidates for RC [9], yet a clear front-runner is the broad category of nanomagnetic devices as their inherent qualities lend themselves to low-power, compact and fast computing. Spatially distributed arrays of interacting nanomagnetic regions provide a framework for defining multiple input and output dimensions, constituting a system whose dimensionality is equal to the number of N structures. Allwood et al. assess the dynamical response of magnetic reservoirs that exploit the damped, oscillatory motion of magnetic moments according to the Laudau-Lifshitz-Gilbert equation of motion. With frequencies in the Megahertz to Terahertz region and settling times in the order of nanoseconds, ferromagnetic materials are not only well suited to high-speed applications, but naturally satisfy the ESP. In summary, they can be treated as "non-linear activation functions with short-term temporal dependencies" [10]. The validity of this appraisal has been corroborated by simulation work by Dale et al. In the study, a thin magnetic ferromagnetic film divided into macro-regions was simulated in software as the reservoir for an RC implementation [11]. The group demonstrated that simulated thin-films of copper, iron & cobalt of various area and thickness can be used successfully to predict a triumvirate of complex industry standard prediction tasks: Santa Fe Laser, NARMA-10 and NARMA-30. The study found that the materials were competitive against neural networks and typically outperformed them when the reservoir size was small.

Design choices are notoriously hard to justify in RC, with little concrete theory and scarce

heuristics for optimising reservoir parameters to best perform a specific task. Qualitative appraisals of behaviour exist, providing a pathway for justified system implementation parameters by virtue of analogous use cases. In light of this, I will be basing my setup on the "Reservoir Computing with Thin Magnetic Films" paper where appropriate, or where there is no known rule-book for making informed design choices, beyond a qualitative observation of implementation success. Efforts are ongoing to try and formulate an industry standard for bench-marking the *N-dimensional* feature space of substrates, such as the CHARC framework proposed by researchers at the University of York in the UK [12]. Common metrics for feature-space evaluation are Kernel Rank, Generalisation Rank and Linear Memory Capacity, although other measures have been considered such as Shannon Entropy and N^{th} Order Memory Capacity. Others have shown that a computational learning approach could constitute a new paradigm for choosing configurable reservoir parameters. Hermans et al. have demonstrated that backpropagation training is achievable even with a physical medium [13], forming the basis for a substrate optimisation framework called evolution *in materio* [14]. Electronically controlling modifiable system parameters during the training phase could optimise the proposed biosensor for pattern recognition of desired magnetic phenomena. Furthermore, performing evolution in a simulation-based setup could provide optimisation of topological design choices, such as layout, physical dimensions and chemistry of the substrate's constituent parts or regions.

The literature on how to separate testing and training data is varied, especially between system architectures. Many opt for a static split, determined heuristically based on the relative size of the datasets utilised. To remove the guesswork where possible, using a cross-validation splitting algorithm has shown to find near-optimal solutions and consistent greater accuracy than other statistical approaches [15]. The output layer neurons are still required to be physical devices, or metaphysical software implementations. They are therefore highly configurable and should be optimised for their use-case. Naturally, a sizeable host of neuron activation functions have been trialled, with differing trade-offs, typically between complexity and computational overhead [16]. The desired data for this project would be open source time-series of magnetic field properties emanating from physiological or biological phenomena. The distance between two adjacent time-steps will likely be substantial compared with the nanosecond dynamics of the simulated substrate. As such, due consideration is required for how the data will be presented in the simulation work. Furthermore, a physical device would require analogue to digital conversion of captured magnetic data. It is important to understand how quantisation of continuous data affects pattern recognition and if any techniques, such as linear or polynomial interpolation,

could improve the systems performance. Moreover, The speed of the substrate dynamics is secondary to the speed of the sampling apparatus in a physical device. In simulation this isn't an issue, but it becomes important when discussing a real-world implementation.

3.2 Nanostructure Simulation

As previously mentioned, Dale et al. successfully simulated a thin magnetic film structure and demonstrated its efficacy in an RC setup. The atomistic simulator they used is a state-of-the-art software developed at the University of York, capable of calculating complex and largely unexplored interactions, such as antiferromagnetic exchange interactions, called Vampire [17]. The complex dynamics of magnetic materials stem from the interference effects of collective excitations of the constituent domains which, if phase-coherent, are called spin-waves. This phenomenon is observed when the material is driven at microwave frequencies and constitutes, within this operating regime, a magnonic device, named after the quasi-particle of the spin-wave: the magnon [10]. It may be unlikely that any physiological mechanisms produce fluctuating fields of such high frequency, yet to ignore this possibility could veil important patterns within the data. It is important therefore to ensure that these dynamics can be captured in simulation. In light of this, an understanding of candidate material properties should include exchange interactions, spin-wave stiffness constants and curie temperatures. Exchange interaction is especially important, as it is the principle quantum mechanism that causes ferromagnetism in transition metals [18]. In "Reservoir computing with thin-film ferromagnetic devices" [11], the choice of materials was corroborated by robust knowledge of these properties from *ab initio* extrapolation by Pajda et al. [19]. Studies have assessed these properties in other magnetic materials, providing a panoply of potential substrates whose magnetic behaviour can be accurately captured at the nanoscale [20, 21, 22]. The methodology of [11] precludes substrate performance at or above room temperature; any use-case operating in a human-biology environment is unexplored territory, and it is unknown whether the thermal effects can be overcome by the system. Their findings conclude that the performance of copper was least affected by increased simulation temperature, and could be a good starting point for exploration of this feasibility study.

Figure 2 shows a visual representation of the thin-film architecture, its division into macro-cells and resulting array of magnetic polarisations that will serve as the reservoir output. The 2D profile of the macro-cells is purely arbitrary and there is no stringent requirement for these

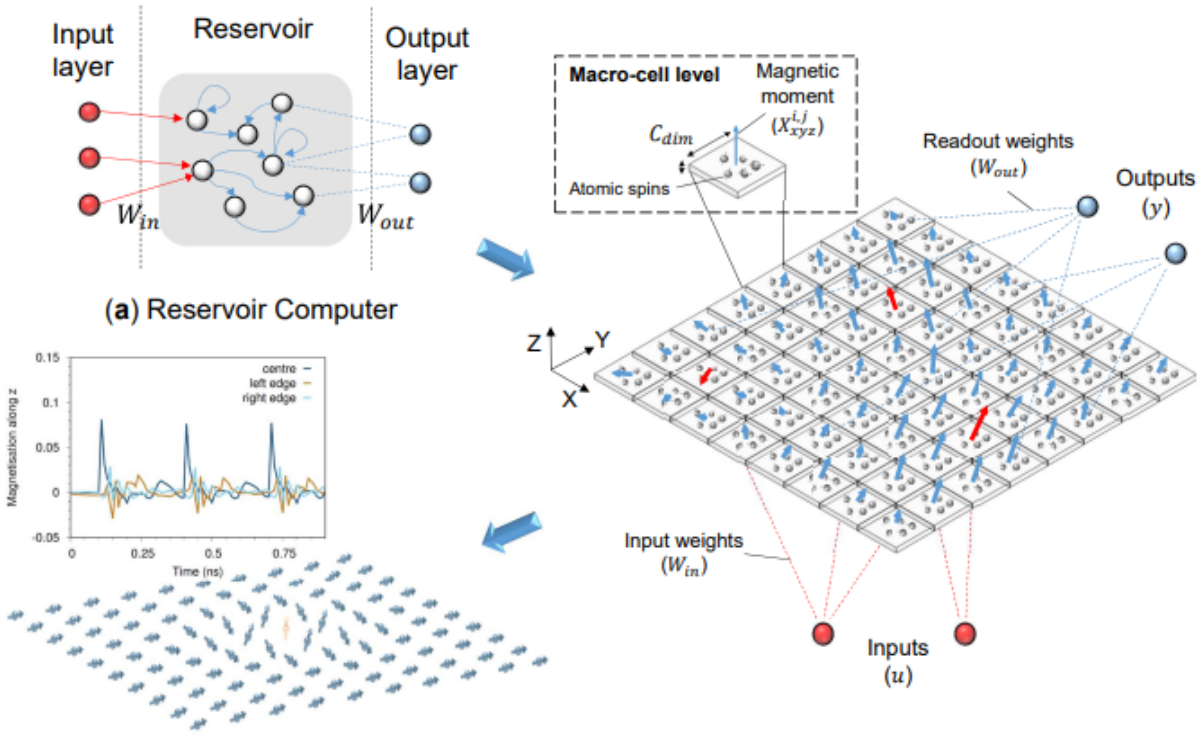

Figure 2: Simulation setup as described in "Reservoir Computing with Thin Magnetic Films" [11]. The thin-film is divided into macro-cells whose state parameter is the magnetic polarisation vectory, as a function of x,y,z field components.

to have square geometry. This topology represents the simplest representation of regional domains, yet any other polygon is feasible, at the cost of greater mathematical complexity. The separation between domains could also be physical rather than purely spatial, with each cell a separate magnetic mesa separated by space or a non-magnetic spacer material. However, such an assembly would have to be carefully constructed so that the distance between panels doesn't destroy the inter-connectivity or high-dimensionality of the reservoir dynamics. A study by the University of Sheffield demonstrated the efficacy of an array of magnetic rings as a reservoir [23]. The group physically built the device using E-beam lithography and tested several permutations of domain separation paradigms and system architectures. Each explored implementation exhibited state-of-the-art performance and proved optimised to a particular subset of input dynamics. Physical demonstrations are rare and could be an ideal basis from which to build a valid framework for this project.

Dale et al.'s methodology entailed inducing a localised magnetic field in every single macro-cells by means of an input current, modulated by an input weight matrix [11]. Similarly, each polarisation vector is passed via weighted connection to a node in the output layer. Optimising the setup for my use-case will have to explore different connection schemes between reservoir

and output layer, as well as how to provide the inputs to system in such a way as to maximise fidelity to a real-world scenario.

3.3 Biological Compatibility

If the results of this feasibility study conclude that the concept shows sufficient promise to warrant further exploration, integration with *in-situ* physiology cannot be ignored. Either through choice of materials, or appropriate shielding, the device must not present non-negligible toxicity or invasiveness for the concept to be a clinical and commercial success. The likelihood is that in a successful setup the device will require such proximity to the associated biology that, in the scenario of a human diagnostic sensor, it will require implanting, at the very least on a sub-dermal level. Direct contact with tissue presents significant concerns with regards to metallic poisoning, especially if the device materials can dissolve and spread into the surrounding area or, in a worst case scenario, the blood stream. A study found that oral consumption of a mere $6mg$ of copper per 1 litre of water in enough to cause adverse effects in humans, and that chronic overexposure can cause liver damage [24]. Furthermore, recent work has shown that nano-particles of copper oxide present serious levels of genotoxicity, cytotoxicity and immunotoxicity [25]. It is a similar story with other ferromagnetic materials: overexposure to cobalt, for example in metal-on-metal hip implants, has been linked to neurological, cardiovascular and endocrine deficits [26]. A mere $300\mu g/l$ in the bloodstream can cause adverse effects in adults. Even iron, a fundamental element for our biology, can cause toxicology and mutagenic concerns at the cellular level when present as iron-oxide [27]. A physical device based on any of these compounds would need to ensure that nano-particles cannot leech into the surrounding tissue, nor form dangerous oxides, which besides compromising the efficacy and longevity of the device, could heighten the associated toxicological risks. Due consideration is required in designing a housing assembly that can mitigate these risks and not introduce it's own bio-compatibility concerns. Parylene is a polymer discovered in the 40s that has been extensively used for coating sub-dermal chips in animals. As the ethical landscape surrounding human implantation evolves, parylene and derivatives are being explored for biomedical devices [28]. The polymer has seen extensive use in coating electronic components, a notable case being ferrite rings used in magnetic core memory - the main RAM memory used on the space shuttle. This triple compatibility with electronics, magnetics and biology, coupled with inherent anticorrosive and antibacterial properties, makes parylene a highly desirable material for the proposed biosensor concept.

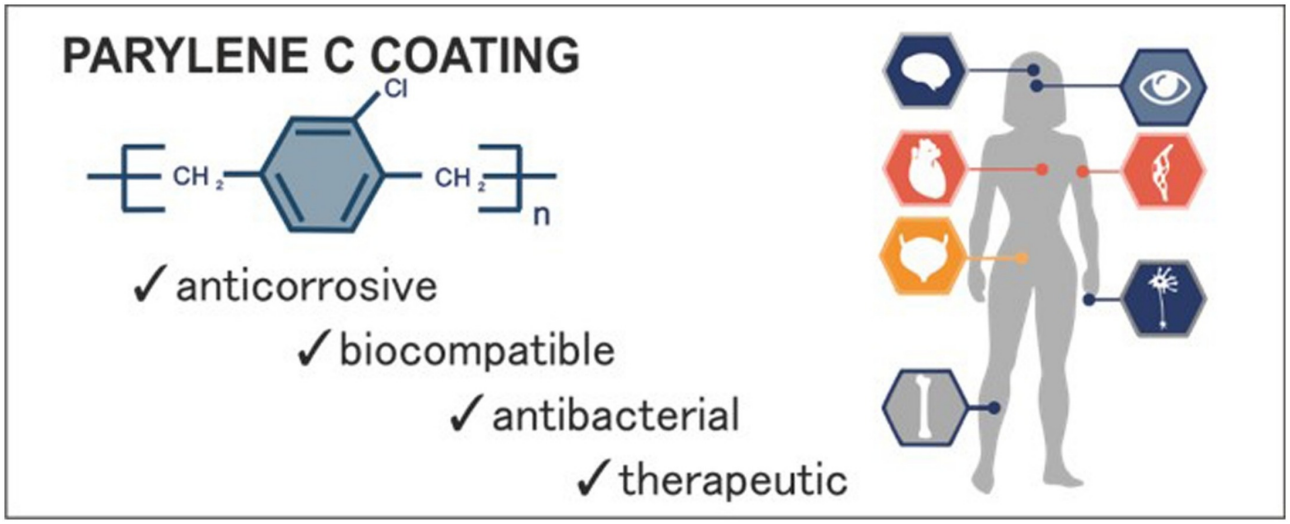

Figure 3: Parylene has seen extensive use since its discovery in 1947 in industries such as electronics, magnetics and veterinary implants. It is suitable for a host of biomedical applications and boasts unparalleled compatibility with many different parts of the human anatomy [28].

The nanoscale size of the proposed device naturally lends itself to *in-situ* implantation. As with any intra-anatomical device, especially one which may provide augmentation rather than performing a life-critical role, an onus on being minimally invasive is both desirable and ethical. While there isn't a strict numerical threshold universally agreed upon for what constitutes "minimally invasive", an accepted definition is any technique that achieves the same surgical objectives as traditional open surgery but with smaller incisions, reduced tissue trauma, and faster recovery times [29]. Dale et al.'s simulated thin-film's largest dimension did not exceed fractions of a micrometre; coupling this with modern IC technology capable of $3nm$ transistors, promises a very small scale device indeed. One can safely assume that in a state-of-the-art implementation of this concept the vast majority of the device volume would stem from the sensor's power supply, probably in the form of a battery. Existing implantable devices are typically on the millimetre scale, providing substantial room for scalability in the context of nanoscale devices. For comparison, progesterone-releasing sub-dermal contraceptive implants are typically 40–$44mm$ long and 2.0–$2.5mm$ in diameter [30]. As a like-for-like example, a study exploring an electronically-controlled sub-dermal drug release system achieved device dimensions of $54mm \times 31mm \times 11mm$ [31]. The PCB itself is a slight $13.0mm \times 5.4mm \times 0.5mm$, the battery being responsible for the remaining bulk.

4 Implementation Strategies

I have specified three tiers of implementation, the first being the simplest scope of a complete successful project and the others constituting going "above and beyond", but not integral to the definition of success. It is important to note that I have structured the tiers system such that any features from tiers 2 & 3 can be cherry-picked arbitrarily and incorporated into the project.

4.1 Tier 1: Basic Functionality

The definition of success for this project is to either prove or disprove the basic functionality of the concept, by answering the question: "using real magneto-medical datasets as an input to a simulated thin magnetic film, is it possible to train a software-based output layer of perceptrons to infer the input field trace, or recognise patterns therein?". From a setup perspective, the three main challenges are:

- *Acquire and translate input data*: for any assessment of feasibility to be valid, the input data has to be an accurate representation of real physiological phenomena. Furthermore, it needs to be input to the system in such a way as to closely mimic real-world dynamics.

- *Simulate substrate*: a basic requirement for this project is, in a first instance, generating the crystalline lattice structure. Once this has been achieved, a test script will need to simulate the reaction to an input and to output an array of magnetic polarisations. These will subsequently need to be averaged over each macro-cell area to reduce the size and increase interpretability of the dataset, as well as restrict the computational overhead in the output layer stage.

- *Emulate and train perceptron layer*: an array of neurons will need to be instantiated and connections mapped to the input data. Ridge regression training has to successfully modify the output weights. The output from the perceptron array needs to construct an output matrix that is clearly interpretable.

- *Biological compatibility*: a deep dive into the design choices and strategies to be considered for such a device to not alter or influence the target physiology. The premise of the project

is ultimately futile unless the technology can be made compatible with biological systems.

Once this framework has been successfully implemented, the project can begin in earnest. The goal is to trial as many different datasets, preferably from physiologically diverse mechanisms. The simplest form of test is to split the data into training and test sets and to try and forecast the test set. Accuracy scores can be calculated to assess the closeness of the prediction. Considerations such as output layer activation function, reservoir-output connectivity, input-reservoir connectivity and any causally resulting features, such as output node count, can be swept to assess performance with different tasks. By heuristic iteration, I can try and get close to an optimal implementation. Two performance metrics can be explored: specific task proficiency and ability to generalise between either different datasets of the same magnetic phenomenon, or altogether different physiological mechanisms.

4.2 Tier 2: Nanomagnetic Exploration

Building on the base premise of 4.1, the features stated in this section are supplemental to the original definition of success, but also represent an optimal implementation of the project. These are the main areas of development:

- *In-materio evolution*: taking inspiration from Dale et al., an evolutionary algorithm could be used to find the optimal nanostructure parameters for each assessed material, for a specific dataset [11]. Using this method would result in more exhaustive findings and reduce reliance on the quality of my exploratory premonitions.

- *Multiple thin-film geometries*: alongside the square film geometry, different topologies could be tested, such as annular, triangular, circular islands etc.

4.3 Tier 3: Road to Realisation

The features listed in this section would render the project universally complete, by projecting the continuation of the endeavour, speculating on various aspects of future work that would build on the premise of my efforts. Important considerations include:

- *Physical test strategy*: advice could be proffered on how to proceed with physical testing, from epitaxial growth of the film, to chip-based output layer architecture.

- *Manufacturing*: A generic assessment of the manufacturing process and equipment, using a holistic approach to describe a conjectured guise of the sensor and the main technologies employed.

- *Commercialisation*: considerations for achieving a happy medium between cost, performance and safety. How the composition and size of both nanolayer and perceptron array change when cost is taken into account. An appraisal of how many units would need to be manufactured and sold to guarantee a realistic price whilst covering costs.

5 Timetable

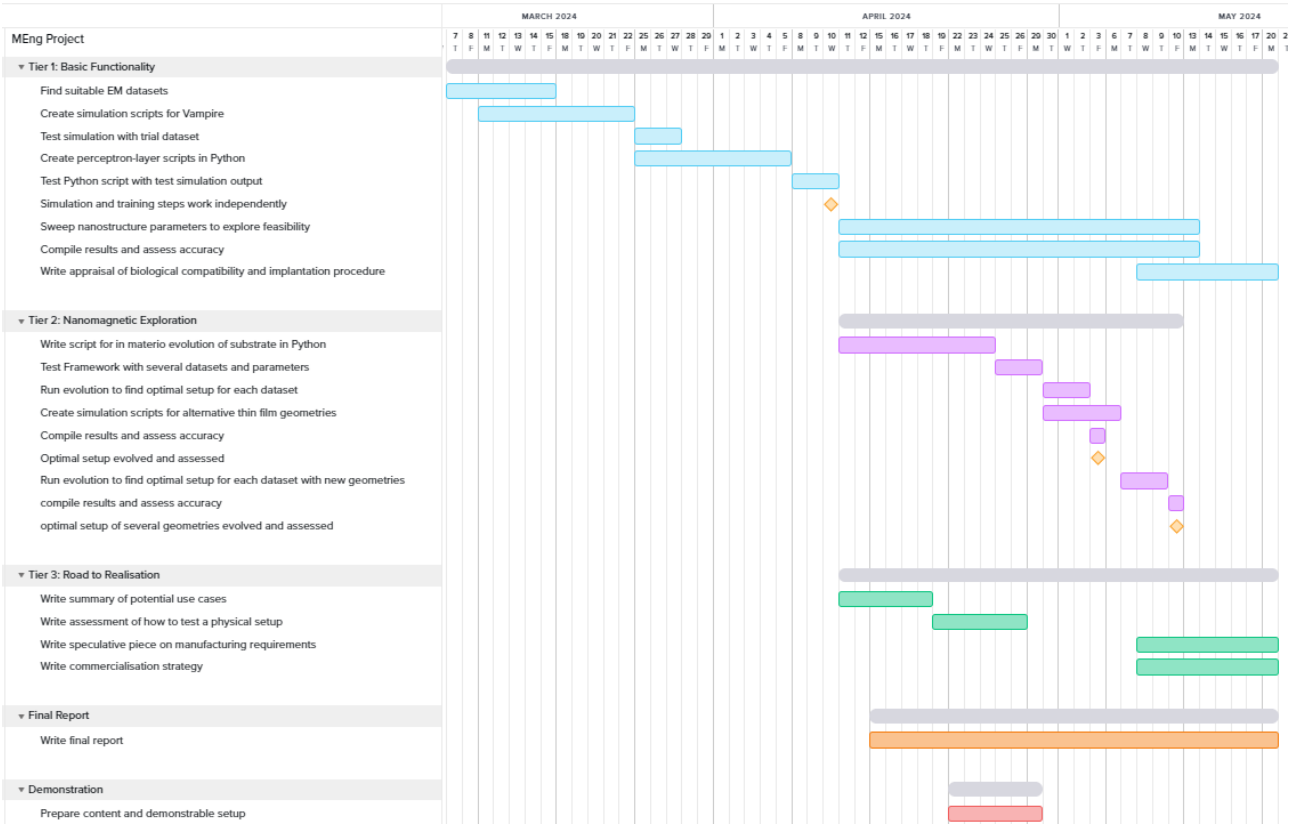

Figure 4: Projected Development Timeline of Project. The stated timelines for tiers 2 & 3 only apply *if* those elements are incorporated into the project. This gantt chart represents an ideal roll-out schedule and could change as the project requirements evolve.

6 Closing Statement

In conclusion, this project represents an exciting exploration into the feasibility of utilising thin magnetic films as reservoirs within the framework of Reservoir Computing, a cutting-edge machine learning paradigm. By leveraging the inherent properties of physical substrates, the ultimate aim is to conceptualise minimally invasive, low-power biosensors capable of discerning subtle changes in fundamental states of physiological processes. By harnessing the power of the University of York's in-house atomistic simulator, Vampire, and the flexibility of the high-level programming language Python, I believe a compelling case can be made for the viability of such an implementation. By demonstrating the validity of the underlying physics and technologies, I aim to lay the groundwork for future research into this particular use-case, marrying unconventional computing with nanotechnology in a biological context.

6.1 Statement on Ethics

The project is entirely software based, any and all stated physical design considerations are academically informed conjecture or speculation. Discussion on biological compatibility will adhere strictly and exclusively to scientific concerns. In light of these facts there are no ethical considerations that need to be stated.

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