

## Research Statement

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My work strongly relies on providing well-designed schemes, techniques, algorithms, protocols, languages, compilers, CAD tools, mathematical theories, and solutions to solve problems in science, engineering, and medicine, and to improve the performance of computer systems by eliminating unnecessary bottlenecks. My research interests and experience span a wide range of topics in computer science, electrical engineering, applied mathematics and physiology [1-13]. During my PhD at the University of Ulster and followed particularly by my lectureship position at the University of Hertfordshire, I have been intrigued to take advantage of different mathematical concepts and theories to understand the underlying mechanisms governing biological systems. Prior to my PhD, because of the strong interdisciplinary nature of my research, I had developed a rich network of collaborations with researchers in four different laboratories at Shahed University and the Sharif University of Technology, including, High-Performance Computing Centre (HPCC), Integrated Circuits & Systems Lab (ICSL), Semiconductor Device Modelling Lab (SDML), and Parallel & Distributed Systems Lab (PDSL). Below is an overview of my research activities.

**Current Research:** Mathematical modelling and computer simulation are powerful tools whereby we can analyse complex biological systems, particularly, neural phenomena involved in brain dysfunction. Recent studies highlight the importance of increasing our understanding of microglia (a type of neural cell) physiology since their functions play critical roles in both normal physiological and pathological dynamics of the human brain. In addition, a realistic view of the brain models will take place when the interaction between all types of neural cells can be modelled, which is addressed as part of my research efforts. Currently, I am carrying out research on experimental/computational biology, biophysics and human brain physiology in close collaboration with experimental neuroscientists from the University of Reading in the School of Pharmacy to get deeper, more than realistic insight into the human brain in my models within the following areas [11-14]:

- To construct a three-dimensional mathematical model of the human brain for studying the interaction of neurons with other brain cells like glial cells by utilising human neurophysiology, partial differential equations, numerical analysis and supercomputers.
- To Make a realistic cellular model of the human neuroimmune system using experimental techniques and electrophysiology.
- To study the underlying neuroinflammatory pathways implicated in neurodegeneration (Alzheimer's and Parkinson's diseases).

My final goal is to provide a unified computational framework for the neuroscience community to study human brain diseases at a cellular level by exploiting the power of cutting-edge supercomputers.

## **Past Research (without any priority order)**

### **A. Computational Neuroscience**

During my PhD studies at Ulster University working on my thesis, my main goal was to develop new mathematical models for the key agents that regulate microglial functions such as agonist-mediated P2X/P2Y calcium signalling transduction and actin polymerisation towards microglial motility [11]. I have built several mathematical models for different aspects of microglial physiology<sup>1</sup>. Due to the interdisciplinary nature of my field, I had to study several medical prerequisites to gain a deep understanding of the research (including, biology, biochemistry, human physiology, neuroscience, mathematical physiology, and glial neurobiology). The models are expressed as sets of a system of non-linear ordinary differential equations (ODEs) that must be fitted to experimentally electrophysiological data. The models were developed from scratch because of the complexity of human biophysical data. In two of the models, Hodgkin–Huxley (HH) formalism is directly extended to mathematically model biophysical processes beyond action potentials for the first time. Parameter estimation and curve fitting (a fundamental optimisation problem) play a key role in all models developed. Therefore, I have developed deep knowledge in numerical optimisation, particularly, multi-objective and stochastic optimisation. In a nutshell, the predictions provided by the models reveal new quantitative insights into how microglia regulate ionic concentrations and motility in terms of physiological interactions and transient responses.

### **B. Distributed Systems and High-Performance Computing (HPC)**

I have carried out long-standing research to build several distributed middleware for Grid and Cloud Computing from .NET Framework in C#<sup>2</sup> to native code in C/C++ [3-10]. Recently, I have completed a unified software infrastructure, called Parvicursor<sup>3</sup>, to facilitate the design of Grid and Cloud Computing. Parvicursor infrastructure is a middleware system grounded on a specialised concept of distributed objects and native ECMA.NET-compliant execution for highly concurrent distributed systems, and to make writing middleware easier on heterogeneous platforms. It takes care of low-level network programming interfaces for Grid/Cloud-specific platforms and allows the middleware architects to focus their efforts on their middleware logic with the help of the integrated, scalable Parvicursor Execution System (PES) which implements an extensible plugin software design pattern to support multiple, pluggable server-side services. Parvicursor.NET Framework is the first attempt that allows developers to implement .NET-based programs directly in native code. Parvicursor makes use of combining thread-level parallelism and

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<sup>1</sup> <https://github.com/poshtkohi/computational-neuroscience>

<sup>2</sup> <https://github.com/poshtkohi/dotgrid>

<sup>3</sup> <https://github.com/poshtkohi/pads>

distributed memory programming models to exploit the strengths of both models in the many-core era. xThread provides the capability of transparent distributed shared memory remote code execution, dynamic distributed object registration and activation, distributed operation dispatching, checkpoint/restore, etc. xDFS proposes utilities and libraries for transmitting, storing and managing massive data sets over LANs, WANs and the Internet.

In [4], my work focuses on resource allocation and discovery algorithms for distributed systems. A new optimistic synchronisation algorithm is presented in [1] by mixing multiple synchronisation protocols that is applicable to many existing synchronisation algorithms in parallel computing (this is a work-in-progress to generalise a universal synchronisation algorithm for distributed systems with its many applications to HPC, parallel programming languages, parallel numerical algorithms and so forth; please see Section 'Future Research'). Moreover, I have written many parallel programs based on message passing interface (MPI) and thread programming style (and hybrid MPI/Thread) in C/C++/FORTRAN for computational physics and electronics, scientific computing, and distributed systems.

### **C. Programming Languages and Compilers, and Advanced Computer Modelling & Simulation**

Programming languages have been one of my primary motivations towards computer science. I have a deep understanding of the modelling and simulation of discrete-event, continuous-time and dynamical systems. I have been working on Parallel Discrete Event Simulation (PDES)<sup>1</sup> and thus I developed a new object-oriented, hierarchical, component-based optimistic parallel programming and simulation language, called OSML, for modelling and simulation of extreme-scale parallel computer architectures and embedded systems on many-core hosts and supercomputers [1]. This language is accompanied by a UML toolset and a comprehensive compiler suite written in C++ with LLVM/Clang. This language is also a kind of reversible programming language and can be used as a replacement for parallel simulation of existing System-Level Description Languages (SLDLs) and Hardware Description Languages (HDLs) like SystemC, Verilog, DEVS and NS2. The key contributions of this research, for the first time, are as follows [1]: (a) OSML solves one of the six major research challenges in the Parallel and Distributed Simulation (PADS) community—making PADS widely accessible and simplifying the model development through Cloud Computing, (b) it applies optimistic PDES to SLDLs, (c) it allows different hardware or computer models at different electronic abstraction levels to be executed by optimistic synchronisation, including, many-state processors, memories, buses, routers, and so on. This is achieved by proposing a hybrid state-saving scheme for optimistic execution, (d) two PDES's systems programming and application programming models are precisely defined, and finally (e) OSML provides cross-language interoperability among multiple simulation languages through language compilers and tools for co-simulation.

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<sup>1</sup> <https://github.com/poshtkohi/pdes>

A conservative parallel system modelling and simulation language, called PSML<sup>1</sup>, is introduced in [2] with a myriad of multi-core optimisations, including, a NUMA-and-hardware-type-aware memory allocator for parallel simulation, zero-copy communication, multi-level thread scheduling, and enhanced deadlock detection and recovery protocol. PSML identifies multiple obstacles for parallelising SLDLs at the electronic system level (ESL) and proposes comprehensive solutions such as memory coherency protocols to support the shared state. The PSML syntax is derived from the C# language and the Parvicursor platform. I have a good familiarity with formal specification and mathematical modelling of parallel programming languages such as Structural Operational Semantics (SOS) and Process Algebra. I benefited from them to formally define the PSML's parallel execution semantics on a PDES abstract machine [2].

Finally, applying parallel simulation to different real-world scenarios, especially extreme-scale neural models, modelling high-performance parallel distributed computers, computer networks and Cloud Computing are my other research topics [1].

#### **D. Computer Networks and Big Data**

I designed and implemented a large number of network protocols, particularly, a high-throughput file transfer protocol called DotDFS/xDFS for Big Data applications in Grid and Cloud environments in contrast to the de-facto GridFTP protocol [3, 5, 7, 10]. For the first time, xDFS suggests a concurrent file transfer protocol that simultaneously employs threaded and event-driven models at the protocol level to significantly improve performance and throughput. I have implemented a wide range of parallel I/O mechanisms for this protocol. In [5], an interpolation-based model of multi-stream TCP throughput on WANs is presented. A highly concurrent, asynchronous parallel network programming language is proposed in [3] for many-core processors<sup>2</sup>. During my BSc thesis, I implemented a highly scalable Email service supporting multiple Internet protocols such as SMTP, MIME, POP3 and IMAP4 with a web interface<sup>3</sup>. In this regard, I am interested in Remote Direct Memory Access (RDMA) applications and network protocol design and implementation for high-speed interconnect networks such as InfiniBand over WANs.

#### **E. Operating Systems**

I have developed several kernel-space components for HPC in Linux [3], called zero-copy communication infrastructure (ZCCI), which is meant to improve the efficiency of distributed applications. I took advantage of OS concepts—microkernels and exokernels—to build extensible layered parallel simulation kernels in [1]. One of my long-term goals is to design a minimal language-based operating system directly

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<sup>1</sup> <https://github.com/poshtkohi/psml>

<sup>2</sup> <https://tinyurl.com/asynsocket>

<sup>3</sup> <https://github.com/poshtkohi/pmail>

inside the Linux kernel for HPC and Cloud Computing—I have written the necessary libraries for this exciting project. Overall, I am very interested in many-core operating system design.

## **F. Cryptography and Security**

I have a sound background in symmetric and asymmetric cryptography algorithms, key management and establishment, and attacks on a symmetric key. I developed a lightweight secure transport protocol called xSec [3, 5]. xSec introduces techniques for the authentication of users and secure communication. All Parvicursor services are implemented on xSec's transmission security layer (TSI). This protocol also takes care of high-end servers and low-end mobile devices for cryptography operations. Furthermore, I made use of this protocol to build a striped, secure high-throughput file transfer system optimized for many-core machines in the Grid and Cloud [3]. I am very interested to implement such compute-intensive tasks on accelerators like GPUs and FPGAs. A cryptographic accelerator in Grid environments is reported in [6, 8] for petascale data storage.

## **G. Applied Mathematics and Computational Electronics**

I have a strong background in applied mathematics because of my work at SDML. My research lies in the field of partial differential equations (PDEs), parallel scientific computing, computational mathematics, matrix functions, Padé-derived approximants, numerical analysis, and numerical optimisation. The overall goal of my research is to (a) design novel, efficient and accurate parallel numerical algorithms which take advantage of the inherent structures of mathematical and physical problems, and (b) develop stable and general parallel computational tools which are applicable to a wide range of challenging applications in science and engineering. I have worked with advanced numerical techniques for solving mixed-signal, Multiphysics and scientific computing problems in circuit and system theory, and nanoscale semiconductor devices: ordinary differential equations (ODEs) in state-space equation formalism, and nonlinear PDEs including time-domain finite difference, finite element methods, coupled Schrödinger-Poisson solvers, Boltzmann transport equation, and coupled quantum Monte-Carlo algorithms. Also, I have a good knowledge of device modelling and simulation (TCAD), solid-state physics, electronic transport phenomena, and semiconductor devices, together with a good basis in quantum mechanics<sup>1</sup>.

I have developed a novel spacetime-parallel numerical stiff PDE solver using exponential integrators to be used in supercomputers for large-scale intensive computational problems. I developed the entire theory of this new approach from scratch, including, the action of a matrix exponential upon a vector, preconditioner, and time-parallel numerical integration methods. Subsequently, I will be building the spacetime-parallel numerical simulator for ODEs/PDEs in C++ and MPI. More information about this

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<sup>1</sup> <https://github.com/poshtkoi/computational-physics>

project in conjunction with its basis on matrix functions and my works in computational electronics is available upon request.

## **H. Computer-Aided Design (CAD) for Electronic Design Automation (EDA)**

I have developed several CAD tools, called Troodon, for modelling, simulation, visualisation, and power-performance evaluation of digital and analogue electronics systems on Cloud platforms in ICSL [1, 2]. Designers write their model's blueprint using one of the hardware description languages such as OSML, SystemC and UML. They are connected to the Cloud-based Troodon tool through a browser and do their time-consuming simulation tasks. In addition, I have designed different GUI-based CAD tools for analogue circuit design in Java and Eclipse and implemented the underlying mathematical modelling formulas<sup>1</sup>.

## **I. Computer Architecture**

I have a solid background in digital hardware design (e.g., SystemC, Verilog, VLSI, low-power circuit design, FPGA and ARM), high-level synthesis (HLS), HW/SW co-design, place and route, and working with CAD tools for synthesising a complete HW blueprint from system to transistor implementation [1, 2]. Furthermore, during writing my first book [10], I did read many papers and texts regarding advanced computing including textbooks on advanced computer architecture, transactional memory, virtualisation and GPU computing, and developed new materials reliant on these concepts (e.g., multiple novel lock-free algorithms [10]). Based on my graduate background in system-on-chip design and VLSI, I am using these concepts day to day to prepare materials for ongoing publications. From this perspective, I am very interested in researching novel computer architectures, for example, exascale computers, optical and biological computing, and quantum computers.

## **J. My First Book**

I wrote a book on parallel and distributed systems [10] with Taylor & Francis/CRC Press, USA<sup>2</sup>. This book spans my obtained experience over many years of research and development to build different distributed middleware components, particularly in Grid and Cloud Computing. It teaches the reader how to construct a complex distributed software infrastructure from the ground up. The book arrives at a critical time when Moore's Law is fading, and the development of distributed systems and high-performance computing is of unprecedented demand and importance. The book aims to convey necessary knowledge, principles, and software practices that underlie the development of a vast majority of parallel and distributed systems, particularly Grid/Cloud Computing and supercomputers. Advanced topics relevant to computer architecture, operating systems, and parallel programming techniques and models for many-core processors, supercomputers and computer networks are provided to allow readers in order to gain

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<sup>1</sup> <https://github.com/poshtkohi/jpad>

<sup>2</sup> <https://github.com/poshtkohi/pads>

incremental experience to implement their own platforms from scratch. The text helps readers gradually think parallel through a programming language that had been primarily intended to model distributed systems!

**Future Research:** I have planned several future extensions to my previous works. Firstly, as the HH model has been turned into a *de facto* basis in biophysics, one of my grand goals is to develop an elegant mathematical framework where a generalised HH formalism can be used to capture multiple data sets obtained by a wide range of electrophysiological experiments. This project requires building multiple relevant mathematical models for different biophysical problems and finding the best candidate models. Of course, parameter estimation is an important matter here because many biochemical experiments allow us to have access to a few observables. I have found out that curve fitting is an art to science since existing parameter estimation frameworks fail to effectively find the global extrema of the underlying loss functions. Alternative optimisation strategies must be explored or developed for complex biophysical data. Secondly, since I proposed a hybrid optimistic synchronisation algorithm in [1] applied to parallel simulation languages, I want to generalise it to non-simulation parallel programming languages by providing a unified parallel programming and simulation language which is of paramount importance in the era of exascale computing. Thirdly, another plan is to design a sandboxing infrastructure to achieve the features available in the Code Access Security (CAS) model of the .NET Framework and ECMA.NET standard in the native Parvicursor infrastructure. This will open new insights into the design of Cloud infrastructures without the need for resource-intensive virtualisation techniques like hypervisors and increase the performance as possible as close to the efficiency of native code [3]. Fourthly, I am going to expand my research into extreme-scale SSD/InfiniBand-based network computing and deep learning. I will implement a unified parallel network programming language and benefit from probability theory and deep learning to optimise the language runtime parameters. Fifthly, before my PhD studies, I was developing a unified parallel Multiphysics modelling and simulation language called OSML-AMS (Analogue-Mixed Signal) using an assortment of optimistic PDES, domain decomposition and exponential integrators to handle multi-scale spatial regions. This is a work-in-progress project that will be resumed in the future. Sixthly, I have been designing a parallel SPICE-like simulator based on chaotic iterations and optimistic PDES from scratch for analogue circuits and its applications to neuroscience modelling for brain research on supercomputers.



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