Ali Rezaei, Ph.D.

Physics • Quantum Computing • HPC Engineering • Device Simulation • TCAD

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Profiles: LinkedIn | Google Scholar | ResearchGate | RoaRQ Team | Online CV

Summary

- Physicist and research software engineer with 5+ years of experience in quantum simulation, high-performance computing (HPC), and nanoelectronic device modelling (TCAD).
- Developer of scalable, high-performance simulation tools, including open-source tools such as QuEST (quantum circuit simulator) and NESS (NEGF-based TCAD framework).
- Expert in performance-portable HPC, from low-level kernel optimisation to efficient algorithms and data structures. Proficient with profiling, cache-aware memory layouts, custom scheduling, MPI/OpenMP parallelisation, heterogeneous acceleration, and reproducible, containerised pipelines.
- Experienced program manager of multi-year R&D projects across academia and industry, with strengths in Agile leadership, milestone tracking, stakeholder coordination, and delivery planning.

Skills

- **Programming Languages:** C, C++, Python, Fortran
- **HPC & Parallelism:** MPI, OpenMP, CUDA, SIMD (SSE/AVX/AVX-512), hybrid CPU-GPU execution, NUMA-aware optimisation, hardware-aware tuning, Slurm
- **Profiling & Performance:** Intel VTune, Memory Latency Checker, Intel PCM, Valgrind, Linux perf, likwid
- **Quantum SDKs & Libraries:** QuEST (co-developer), Qiskit, Pennylane, cuQuantum, QuESTlink
- **Scientific Toolkits:** NumPy, SciPy, SymPy, Pandas, MATLAB, Mathematica, JupyterLab, Gnuplot, VTK, ParaView
- **Numerical:** Coupled PDE solvers, finite-difference / finite-volume / finite-element methods, NEGF formalism, linear algebra
- **EDA / TCAD:** NESS (co-developer), Synopsys Sentaurus, Silvaco Atlas, QuantumATK, OMEN, NEMO
- **DevOps & Build Systems:** Linux (HPC CLI, Bash), Git (CI/CD), Docker, Kubernetes, Spack, Conda, CMake, Make, Catch2/CTest
- **IDEs & Editors:** VS Code, Vim, Visual Studio
- **Project & Team Management:** Jira, Gantt charts, MS Project, Agile/Scrum workflows, reporting, documentation
- **Personal:** Analytical, detail-driven, strong problem-solver, effective communicator and team contributor

Education

University of Konstanz, Germany *01/2016 – 12/2019*
Ph.D. in Condensed Matter Physics (Dr. rer. nat.), *Magna cum laude*
Thesis: Non-equilibrium and spin transport in hybrids of superconductors and magnets
Quantum Transport Group – Supervisor: Prof. Dr. Wolfgang Belzig

Institute for Advanced Studies in Basic Sciences, Iran *09/2012 – 04/2015*
M.Sc. in Condensed Matter Physics
Thesis: Thermoelectric properties of 3D topological insulators
Many-body Theory Group – Supervisors: Dr. Saeed Abedinpour, Dr. Jahan Abouie

University of Urmia, Iran *09/2007 – 08/2011*
B.Sc. in Solid State Physics

Experience

Quantum HPC Researcher - QuEST (C/C++), ICSA/EPCC, University of Edinburgh, UK ***02/2024 – Present***

- Implemented a high-performance extension for **QuEST v4**, featuring a new data structure, NUMA-aware design, AVX-512 vectorisation, cache blocking, fused multiply-add, prefetching, and loop unrolling

- Developed a custom task scheduler with memory placement and core pinning, minimising inter-socket latency
- Utilised microarchitectural profilers to identify bottlenecks and iteratively tune performance
- Achieved up to 6.5x speedups in quantum circuit benchmarks on multi-socket CPUs (preprint)
- Published open-source code (repo). Rigorous benchmarking and integration testing in progress, ensuring reliable performance validation across a range of CPU platforms
- Integrating memory tiering (NVMe/CXL), MPI scaling, hybrid CPU-GPU execution, memory compression, and circuit-knitting for enhanced scalability and efficiency
- Supervised 4 MSc/PhD researchers on simulator workflows, debugging practices, and core module development
- Coordinated delivery across multi-partner teams using Jira and Gantt charts. Led stakeholder-facing reporting (EPSRC, RoaRQ, NQCC, Quantum Motion), feedback cycles, and roadmap planning

TCAD Software Developer - NESS (C++), Device Modelling Group, University of Glasgow, UK ***08/2020 – 12/2023***

- Extended the **NESS** TCAD simulator with a scalable NEGF-based quantum transport solver (effective-mass and k.p Hamiltonians) for coupled PDEs (e.g., Poisson–Schrödinger)
- Designed algorithms for quantum tunnelling, statistical variability, effective-mass extraction from ab-initio bands
- Incorporated ML-accelerated NEGF model, achieving 60% convergence speedup while preserving accuracy
- Deployed simulation workflows for NSFETs, FinFETs, planar MOSFETs, and resonant tunnelling diodes. Validated results against IRDS projections using industry-standard TCAD tools
- Optimised for HPC with hybrid MPI/OpenMP parallelism, Docker containers, Git migration, CI/CD pipelines, and unit testing
- Wrote papers, internal documentation, and user tutorials. Supported proposal writing and technical planning
- Managed Agile delivery, and stakeholder reporting for academic–industry collaborations. Coordinated a 10-person team across the codebase and simulation workflows

Ph.D. Candidate, University of Konstanz, Germany ***01/2016 – 12/2019***

- Investigated quantum transport in proximity-coupled superconductor–ferromagnet hybrid devices. Published 3 peer-reviewed papers, contributing to:
  - Triplet Cooper pair generation and control in S/FM spin-valve structures (*first theoretical proposal*)
  - Spin-flip enhanced thermoelectric effects in S/FM junctions (*predicted 5x thermopower boost*)
  - Spin-splitting induced via antiferromagnetic interfaces in superconductors (*first non-FM approach*)
- Coded Fortran solvers for quasiclassical Green's function methods (Eilenberger/Usadel formalism, Nazarov's quantum circuit theory), solving coupled PDEs with self-consistent boundary conditions
- Teaching Assistant for graduate courses:
  - Quantum Field Theory of Nonequilibrium States
  - Advanced Quantum Theory and Electrodynamics
  - Advanced Condensed Matter Physics

Interests

- Quantum computing: algorithms, circuit simulation, error correction, and software tooling
- Nanoelectronic device modelling: TCAD, NEGF, quantum transport, and condensed matter theory
- HPC: parallel programming, architecture-aware optimisation, and scalable CPU/GPU software
- Technical leadership: planning, milestone delivery, stakeholder engagement, and cross-functional coordination

Distinctions

- Graduated *Magna cum laude*, Ph.D. in Condensed Matter Physics – University of Konstanz (Dec 2019)
- Certificate of Training, IRTG Nano (SFB 767) – University of Konstanz, Germany (Dec 2019)
- Best Scientific Poster Prize, 697th WE-Heraeus-Seminar – Physikzentrum Bad Honnef, Germany (Jun 2019)
- Ranked top 0.4% (120 / 30,000+) in the M.Sc. National Physics Entrance Exam – Iran (Sep 2012)

Certifications

- **Project Management: Professional Certificate** (Google)
  Agile/Waterfall, Gantt charts, project lifecycle, Scrum, Kanban, WBS, budgeting, scheduling, RACI, stakeholder coordination
- **IBM Quantum (Qiskit)**
  Variational Algorithm Design, Quantum Algorithms, Quantum Information
- **Proficiency in PennyLane** (pennyLane.ai)
  Basics of quantum programming using PennyLane and hybrid models
- **Amazon Braket Quantum Application Development** (AWS Skill Builder)
- **Machine Learning** (Stanford University)
  Supervised learning (regression, neural networks, SVMs), unsupervised learning (K-means, PCA, anomaly detection), recommender systems, large-scale ML
- **Advanced Data Science with IBM Specialization**
  Scalable Data Science, Advanced Machine Learning and Signal Processing, Applied AI with Deep Learning
- **Data Science Professional Certificate** (IBM)
- Other: **SQL for Data Science** (UC Davis), **Object-Oriented Data Structures in C++** (University of Illinois)

Publications

Quantum Computing & HPC

- Low-Level and NUMA-Aware Optimization for High-Performance Quantum Simulation, *arXiv:2506.09198* (2025)

Semiconductor Devices & TCAD

- Mobility and intrinsic performance of silicon-based nanosheet FETs at 3nm CMOS and beyond, *Solid-State Electronics* **229**, 109172 (2025)
- Analysis of Random Discrete Dopants Embedded Nanowire Resonant Tunnelling Diodes for Generation of Physically Unclonable Functions, *IEEE Trans. Nanotechnology* (2024)
- Predictive Simulation of Nanosheet Transistors Including the Impact of Access Resistance, *IEEE SISPAD* (2024)
- Unravelling the Impact of Random Dopant Fluctuations on Si-based 3nm NSFET: A NEGF Analysis, *IEEE NANO* (2024)
- Study of Electron Mobility in Ultra-scaled Silicon Nanosheet FET, *Physica Scripta* **99**, 075410 (2024)
- Convolutional Machine Learning Method for Accelerating Non-Equilibrium Green's Function Simulations in Nanosheet Transistors, *IEEE Trans. Electron Devices* (2023)
- Charge Dynamics of Amino Acids Detection and the Effect of Steric Hindrance on FinFET-based Electrolyte-Gated Sensor, *Solid-State Electronics* **210**, 108789 (2023)
- Insights into the Ultra-Steep Subthreshold Slope Gate-all-around Feedback-FET for memory and sensing applications, *IEEE NMDC* (2023)
- Electrolyte Gated FET-based Sensing of Immobilised Amphoteric Molecules Including the Variability in Affinity of the Reactive Sites, *IEEE SISPAD* (2023)
- Fully Convolutional Generative Machine Learning method for accelerating Non-Equilibrium Green's Function simulations, *IEEE SISPAD* (2023)
- Hierarchical simulation of nanosheet field effect transistor: NESS flow, *Solid-State Electronics* **199**, 108489 (2023)
- Statistical device simulations of III-V nanowire resonant tunneling diodes as physical unclonable functions source, *Solid-State Electronics* **194**, 108339 (2022)
- Tcad simulation of novel semiconductor devices, *IEEE ASICON* (2021)
- Simulation and modeling of novel electronic device architectures with NESS (nano-electronic simulation software): A modular nano TCAD simulation framework, *Micromachines* **12**, 680 (2021)
- Nano-Electronic Simulation Software (NESS): A Novel Open-Source TCAD Simulation Environment, *JoMM* **3**, 20030407 (2020)

Superconducting Electronics & Spintronics

- Phase-controlled spin and charge currents in superconductor-ferromagnet hybrids, *PRR* **2**, 033336 (2020)
- Spin-flip enhanced thermoelectricity in superconductor-ferromagnet bilayers, *NJP* **20**, 073034 (2018)
- Spin-splitting induced in a superconductor by an anti-ferromagnetic insulator, *PRL* **121**, 247702 (2018)

Topological Materials & Thermoelectrics

- Effect of hexagonal warping on the surface electrical conductivity of a topological insulator, *Proc. 12th Condensed Matter Physics Conference – Physical Society of Iran* (2015)
- Thermoelectric properties of topological insulators doped with impurities, *Proc. 21st IPM Spring School*, Tehran, Iran (2014)