

Aaron Rock Menezes

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Education

BITS Pilani

Grad Date: 05/26

MSc. (Hons.) in Biological Sciences

Goa, India

BEng. (Hons.) in Electronics & Instrumentation (Minor in Data Science in Climate & Health)

Relevant Coursework: Linear Algebra, Probability & Statistics, Applied Statistical Methods, Foundations of Data Science, Machine Learning, Object Oriented Programming, Bioinformatics, Operating Systems

Research Experience

Brown University

Aug 2025 – Present

Visiting Research Fellow

Providence, RI, USA

- Developing **bio-inspired embodied AI agents** for visual perspective-taking, utilizing Reinforcement Learning to model human-like occlusion reasoning in 3D environments.
- Engineered the **VPTnav** data generation pipeline from scratch in **Isaac Lab**; extended the low-level simulation interface to enable unsupported runtime features like dynamic object re-coloring and scaling.
- Optimized simulation throughput, reducing data collection time from **4 days to under 8 hours** (~12x speedup) while decreasing memory usage by **6x**.

Deep Forest Sciences

Dec 2023 – Jul 2025

ML Research Intern

Remote

- Architected end-to-end image preprocessing pipeline for Prithvi **drug discovery platform** and deployed to production for client use, implementing automated object counting and UNet-based segmentation.
- Researched **generation of novel low-k dielectric materials using LLMs** and using Molecular Dynamics and DFT simulations for validation, screening 40+ candidate materials and **reducing screening time by 83% (30+ days to 5 days) with 15-20% success rate**.

DeepChem

Dec 2023 – Present

Open Source Contributor

Remote

- Added 7+ models** including SCScore, UNet, OneFormer, and Protein Language Models to DeepChem with PyTorch, expanding capabilities in synthetic feasibility, segmentation, and protein analysis for 40k+ users.
- Developed **GPU-accelerated parallel ODE solver** infrastructure using PyTorch, enabling highly scalable neural ODE training and inference.
- Optimized image loading pipeline and authored educational tutorials on automated microscopy and cell segmentation, resulting in **10% boost in site traffic**.

APPCAIR, BITS Pilani

Jan 2023 – Present

Undergraduate ML Researcher

Goa, India

- Developed semi-automatic system for molecule generation and retrosynthesis leveraging LLMs (GPT-4, Claude) with logical feedback loops, generating 20+ novel protein inhibitor candidates targeting JAK2 and dopamine beta-hydroxylase (DBH).
- Designed and implemented LSRPI (Location-Specific RNA-Protein Interaction) Transformer-based model to predict residue-level RNA-protein interactions and generate interaction matrices
- Improved XGBoost-based RNA-protein interaction model, achieving 5% accuracy boost and 10% reduction in processing time through optimized preprocessing.

CSIR-Central Electronics Engineering Research Institute

May 2023 – Jul 2023

AI Research Intern

Rajasthan, India

- Conducted exploratory analysis on multi-channel EEG time-series data to extract temporal correlations and developed interactive visualization dashboard.
- Built lightweight CNN classifier with attention mechanisms for real-time EEG finger movement detection, achieving 85% accuracy and F1-score of 0.75.

Projects

- 6-DOF Robotic Arm with RL-Based Digital Twin** | Python, PyTorch, ESP32, OpenCV Jan 2024 – Present
- Designed and built 6-DOF robotic arm using servos, stepper motors, and ESP32 microcontroller with gripper, wrist (pitch/yaw), elbow, shoulder, and rotating base joints.
 - Developed digital twin simulation for RL-based training on object localization and grasping using image and sensor data for movement control and task execution.
- Time-Masked Autoencoders for Fluid Dynamics** | Python, TensorFlow, PyTorch Nov 2023 – Jan 2024
- Collaborated with Imperial College London researchers to study temporal masking in video autoencoders for fluid dynamics simulations.
 - Implemented models predicting up to 20 future frames of Shallow Water simulations with up to 80% input masking, maintaining 80%+ SSIM.
- Mixture of Experts for Named Entity Recognition** | Python, PyTorch, HuggingFace August 2024
- Implemented MoE layer from scratch and integrated into BiLSTM model for CoNLL 2003 NER dataset, achieving 12% accuracy increase and 32% F1-score improvement over baseline.
- Autonomous Rock Detection System for Mars Rover** | Python, TensorFlow, Linux Oct 2022 – Jan 2023
- Led development of computer vision system for autonomous life detection, including transfer learning-based multi-class rock classifier for biological significance assessment.
 - Achieved **2nd place at Anatolian Rover Challenge (Turkey)** and won **Excellence Award at International Rover Challenge (India)**.

Technical Skills

Languages: Python

Frameworks: PyTorch, TensorFlow, Scikit-learn, HuggingFace, IsaacLab, IsaacSim, OpenCV, StableBaselines3, Git, Linux, Docker

Concepts: Deep Learning, Reinforcement Learning, Computer Vision, LLMs, Data Science, OOP

Research Interests: Embodied AI, Multimodal Learning, Computer Vision, Drug Discovery, Computational Biology

Achievements

INSPIRE Scholar, Dept. of Science and Technology, Govt. of India

Awarded to top 1% of science students in Class 12 HSC board exams with scholarship grant to support further studies in science

Google Summer of Code (GSoC) Mentor

Mentoring at DeepChem for Target Conditioned Antibody Sequence Generation Using Protein Language Models

2nd Place at Anatolian Rover Challenge (ARC), Turkey

Led multidisciplinary team of 7 in designing rover for autonomous life detection in extreme terrain

Publications

Compact and Efficient RNA Representations with RNAVec Enable Residue-Level Interaction Mapping

Authors: Aaron R. Menezes, Omkar S. Sathe, Sanket R. Gupte, Aman A. Kattuparambil, Ashwin Srinivasan, Raviprasad Aduri

Novel representation learning approach for residue-level RNA-protein interaction prediction using only primary sequences

In preparation for Nucleic Acids Research (NAR), 2026

Open Source Differentiable ODE Solving Infrastructure

Authors: Rakshit Singh, Aaron R. Menezes, Rida Irfan, Bharath Ramsundar

Accepted at the AAAI Workshop on AI to Accelerate Science and Engineering (AI2ASE), 2024

Open Source Infrastructure for Automatic Cell Segmentation

Authors: Aaron R. Menezes, Bharath Ramsundar

Arxiv Preprint, 2024