

# Stefan Ritchie *Bioinformatician*

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🐙 github.com/stef1949    🔗 Translational Oncology Collaborator (UCL/CRUK)

## 👤 Profile

Detail-oriented bioinformatician (MSc Genetic Manipulation & Molecular Biosciences) with strengths across **AI for omics**, **structural bioinformatics** and **protein dynamics**. I build **reproducible pipelines** (R, Nextflow, Docker, HPC, GCP) and **ML systems** (representation learning, adversarial autoencoders) that translate research into production-ready, well-tested tooling. Proven collaborator with clinicians and academic partners; comfortable owning the full lifecycle from requirements capture to delivery.

## 🧩 Core Competencies

### Immunoinformatics & Structural Bioinformatics

AlphaFold/structure utilisation, homology modelling, docking (SwissDock), PPI features, MD analysis (RMSD/RMSF,  $\Delta G_{\text{bind}}$ ), visualisation (ChimeraX, Blender)

### Protein Dynamics

NAMD (CUDA-accelerated), CHARMM36, TIP3P, PBC handling; protein–ligand workflows end-to-end; comparative binding analysis

### AI/ML for Genomics & Proteins

Python, **PyTorch** (autoencoders, gradient-reversal adversary), representation learning (AAE/VAE), dimensionality reduction, clustering metrics (silhouette, kBET, iLISI/cLISI, PERMANOVA  $R^2$ ); scikit-learn; W&B logging; CUDA AMP

### Pipelines, Data & Cloud

R, Nextflow, Docker/containers, HPC, **Google Cloud Compute; Bioconductor** (SummarizedExperiment), CSV/TSV logCPM matrices; data curation/QA; version control (Git), CI (GitHub Actions)

### Software Engineering

Clean, modular design; unit tests; documentation; stakeholder communication; secure & regulated practice awareness (ISO/UKAS-aligned mindset)

## 📁 Professional Experience

2024 – 2025  
Brighton

### Bioinformatics Research Project (MSc Research Project), *University of Sussex (UCL & Cancer Research UK)*

- Designed **RNA-seq simulation/benchmarking** pipelines evaluating >10 correction methods (ComBat, Harmony, fastMNN, RUVg).
- Built **reproducible workflows** (R + Nextflow in Docker) designed for HPC/Cloud re-runs; automated QC and metric reports (PERMANOVA  $R^2$ , **kBET**, **iLISI/cLISI**, silhouette).
- Delivered analysis and figures (PCA, clustering stability) that **informed translational oncology collaborators**; partnered effectively with UCL/CRUK on requirements and interpretation.
- Delivered reproducible R pipelines now used by peers implementing machine learning, surrogate and empirical methods, along with diagnostic outputs.
- Emphasis on robust, extensible code suitable for integration into production pipelines.

2023 – Present  
Brighton

### Director & Founder, *Richies 3D Ltd*

- Operate a tech-driven SME delivering **scientific models and wearable electronics**, converting ambiguous partner needs into shippable products.
- Engineered **LumiFur** firmware (C++/ESP32, BLE, OTA) and a SwiftUI companion app; practiced full lifecycle ownership from prototyping to release.
- Managed **100+ international orders/year** with process improvements (~30% efficiency), building repeat academic partnerships.
- Business leadership: stakeholder comms, prioritisation, estimation, and quality management.

10/2021 – 11/2023  
Brighton, United Kingdom

### Dispensing Assistant, *Kamsons Pharmacy*






- Strengthened **SOP adherence**, regulatory compliance and clinical data handling—habits transferable to regulated bioinformatics & quality systems.

## 📁 Projects

08/2025 – Present

### HarmonizeNN, *Adversarial Auto-encoder for Batch Correction*

- Unsupervised **adversarial autoencoder** removing batch signal while preserving biology; outputs **corrected logCPM** matrices, latent embeddings, and diagnostics (PCA panels, batch/label silhouettes).
- Built with **PyTorch**; options for HVG selection, mixed precision (**AMP**), gradient-reversal adversary, LR schedulers, and **Weights & Biases** logging; CLI for training/inference; MIT-licensed; tests + repo hygiene.
- Designed for easy integration into bioinformatics pipelines (CSV counts + metadata; robust orientation/ID matching).
- GPU based CUDA accelerated pipeline

09/2024 – Present	<b>GitHub: stef1949/HarmonizeNN</b>  <b>SimBu</b> , <i>Simulations &amp; Benchmarking for Bulk RNA-seq</i>  <ul style="list-style-type: none"> <li>• <b>Reproducible R workflow</b> to generate bulk RNA-seq from single-cell references, inject batch/biology effects, and <b>benchmark correction methods</b> (limma, ComBat/ComBat-Seq, RUVg/RUVs, SVA/SVA-Seq, fastMNN).</li> <li>• Produces <b>SummarizedExperiment</b> outputs (bulk_counts), caches intermediates, and computes metrics (<b>PERMANOVA R<sup>2</sup></b>, <b>kBET</b>, <b>iLISI/cLISI</b>, <b>silhouettes</b>, <b>PC-R<sup>2</sup></b>, <b>DE TPR/FPR</b>); plots PCA/boxplots for reporting.</li> <li>• CI scaffold with <b>GitHub Actions</b>; MIT-licensed.</li> </ul> <a href="https://github.com/stef1949/SimBu">https://github.com/stef1949/SimBu</a> 
08/2025	<b>Electron Orbital Simulator</b> , <i>WebGL/WebGPU Scientific Visualiser</i>  <ul style="list-style-type: none"> <li>• Browser-based orbital visualiser implementing <b>normalized hydrogenic radial functions</b> and <b>real spherical harmonics</b> with <b>WebGL2/WebGPU</b> render paths (CPU Points, GPU, WebGPU).</li> <li>• Importance sampling (inverse-CDF), interactive UI, <b>unit tests</b> and CI; built with modern JS tooling.</li> </ul> <a href="https://github.com/stef1949/Electron-Orbital-Simulator">https://github.com/stef1949/Electron-Orbital-Simulator</a> 
2019 – 2023	<b>Molecular Dynamics Dissertation</b> , <i>Protein–Ligand Binding</i> <ul style="list-style-type: none"> <li>• Conducted <b>molecular dynamics simulations</b> using homology modelling (SWISS-MODEL) and molecular dynamics simulations with <b>NAMD</b> (CUDA) to investigate protein-ligand free-energy binding potentials between <i>danio rerio</i> drSERTaa-Sertraline complexes with <b>CHARMM36/TIP3P</b> → ΔGbind/RMSD analysis → structural visualisation (ChimeraX/Blender).</li> <li>• SSRI–SERT interactions (zebrafish vs human) studied to characterise binding energetic differences and stability; identified residues and conformational behaviours of interest.</li> <li>• Characterisation of binding energetic differences and stability; identified residues and conformational behaviours of interest.</li> <li>• Identified binding hot spots and conformational instabilities with <b>clinical and ecological relevance</b>.</li> <li>• Analysed <b>protein-ligand interactions</b> to explore drug targeting strategies in cancer biology.</li> <li>• Developed transferable skills in <b>HPC use, protein modelling, and reproducible analysis pipelines</b>.</li> <li>• Showcased ability to design <b>end-to-end computational pipelines</b>: sequence retrieval → homology modelling → docking → MD simulation → free energy/RMSD analysis → visualisation.</li> </ul>

## Education

09/2024 – 09/2025 Brighton	<b>MSc Genetic Manipulation &amp; Molecular Biosciences</b> , <i>University of Sussex</i> <ul style="list-style-type: none"> <li>• Focus: Genetic engineering, bioinformatics pipelines, statistical genetics, and rare disease genomics.</li> <li>• Skills developed: PERMANOVA R<sup>2</sup>, kBET, iLISI/cLISI, silhouette analysis, GWAS, meta-analysis, workflow reproducibility.</li> </ul>
2019 – 09/2024 Brighton	<b>BSc Biomedical Sciences</b> , <i>University of Brighton</i> <ul style="list-style-type: none"> <li>• Highlights: homology modelling vs AlphaFold validation; <b>930 ns</b> CUDA-accelerated NAMD; ΔGbind estimation; protein–ligand interaction mapping; 3D structural visualisation; environmental toxicology implications.</li> </ul>
09/2017 – 04/2019 Rochester	<b>A-Levels</b> , <i>Rochester Grammar School for Girls</i> Biology, Chemistry, Mathematics, EPQ
09/2012 – 08/2017 Rochester	<b>GCSE</b> , <i>Sir Joseph Williamson's Mathematical School</i> A*/A grades in Sciences, Computing, Mathematics, English, Geography, DT

## Skills

<b>RNA-seq analysis</b>  <b>C++</b>  <b>C</b>  <b>SPSS</b>  <b>Molecular Dynamics &amp; Structural Bioinformatics</b> NAMD, GROMACS, CHARMM36, TIP3P, RMSD, binding free energy, Ramachandran plots.	<b>Swift UI</b> LumiFur App built using a cross-platform architecture for iOS, MacOS, WatchOS & iPadOS  <b>Google Cloud Compute</b>  <b>CUDA</b>  <b>Molecular dynamics</b> Protein-Ligand Complexes  <b>Protein Modelling &amp; Docking</b> SWISS-MODEL, AlphaFold, ChimeraX, SwissDock, PoseView.	<b>R</b>  <b>Docker</b>  <b>YAML</b>  <b>Neural Network</b>  <b>Computational Toxicology</b> Predictive modelling of SSRI impacts on aquatic species, environmental bioinformatics.	<b>Python</b>  <b>CSS</b>  <b>Bash</b>  <b>Adversarial Autoencoders</b> HarmonizeNN  <b>HPC &amp; GPU Acceleration</b> CUDA-accelerated MD simulations (NAMD, VMD, QwikMD), parallel workflow optimisation.
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## Awards

04/09/2000

### **Spirit of Sussex Gold Award, *Spirit of Sussex***

Recognised for outstanding contribution to university life through academic excellence, community engagement, and cross-disciplinary entrepreneurial innovation.

2018

### **Duke of Edinburgh's Gold Award, *DofE***

Volunteering, skills, and leadership development.

DofE ID no.919064

## Certificates

### **GPhC Pharmacy Assistant**

NVQ Level 2 accreditation covering prescription processing, pharmaceutical stock management, assembling prescribed items, advising on non-prescribed medicines, and supporting pharmacy services in a clinical setting.

### **Essential First Aid**

St. John's Ambulance basic first aid certified

## Languages

English

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## Keywords

**GNNs • Transformers • Gaussian Processes • Generative Modelling • Reinforcement Learning • Protein-structure prediction • PPI features • Cryo-EM/HDX-MS integration (reading) • Spark/Hadoop (concepts) • AWS/Azure (concepts) • TensorFlow (basics) • OpenMM/Rosetta (concepts) (familiarity/learning – for ATS matching) GNNs • Transformers • Gaussian Processes • Generative Modelling • Reinforcement Learning • Protein-structure prediction • PPI features • Cryo-EM/HDX-MS integration (reading) • Spark/Hadoop (concepts) • AWS/Azure (concepts) • TensorFlow/PyTorch (foundational exposure)**