

Hengjian (Henry) Jia

16 years of writing C since the age of 10. 11 years of machine learning starting with CUDA C since 15. From C, to ML, computational medicine, additive and subtractive manufacturing. I don't know everything there is, but I've gotten pretty good at figuring things out.

EXPERIENCE

University of Warwick — *Doctoral Researcher*

December 2022 - Present

- Worked on integrating lightweight ML guidance into large molecular dynamics simulations. Developed a pipeline for rapidly discovering and validating blood brain barrier permeable molecules from a ~110 million corpus of molecules.
- Pipeline focused on detecting BBB permeability using molecular fragments as we discovered that chemistry was more significant than structure for BBB permeability. Then Lipinski's rule of 5 was used to filter for druglike molecules, until a small set of candidates could be identified and simulated with metadynamics.

University of Warwick — *Research Fellow*

August 2023 - April 2024

- Contracted to help in developing a method of accelerating drug design using latent space Bayesian Optimisation

MidJourney — *Machine Learning Engineer*

July 2022 - December 2022

- Contracted to help build generative image models. Worked on early diffusion models with UNet based architectures and CLIP embeddings.

Ultraleap/Leap Motion — *Machine Learning Engineer*

September 2015 - July 2022

- Experimented with at the time cutting edge techniques including deformable convolutions, diagonal weight decomposition, Spatial transformers, GANs/GAN variants, residual/highway networks, quantised networks, cyclic learning rates/superconvergence, style transfer
- Helped to create and develop in house cloud infrastructure pipeline
- Built an accelerated in-house ML framework in barebones CUDA C before the advent of Tensorflow and PyTorch
- Worked on in-house deep learning based visual odometry

RESEARCH PAPERS

Fast, lightweight BBB permeability predictions for molecular design - 2026
In Review for Molecular Systems Design & Engineering - Hengjian Jia, Gabriele C Sosso

Transparent Machine Learning Model to Understand Drug Permeability through the Blood-Brain Barrier - 2024
Journal of Chemical Information and Modelling - Hengjian Jia, Gabriele C Sosso

Investigation into the effectiveness of long short term memory networks for stock price prediction - 2016 -
ArXiv - Hengjian Jia

(+44) 7522162074

henryjia@protonmail.com

<https://henryjia.github.io/>

github.com/henryjia

SKILLS

Deep learning and machine learning engineering

Tensorflow, PyTorch and PyTorch Lightning

High performance GPU programming in CUDA C

C/C++, Python

Molecular dynamics simulations (GROMACS, CharMM-GUI, Plumed2, CGenFF)

Precision Additive and Subtractive Manufacturing

Embedded systems engineering

Remote team working

Teaching, mentoring

Academic Teaching

Analysis 1 & 2

Linear Algebra

Machine Learning

LANGUAGES

British English

Mandarin Chinese

REFERENCES

Available upon request

OPEN SOURCE & PERSONAL PROJECTS

Faster Flow Matching with Minor Component Metadynamics - 2026 -

- This is a work in progress project to explore using metadynamics to accelerate neural network training. Whilst plenty of research exists in the present on utilising machine learning to learn collective variables to aid metadynamics. I was curious as if the converse could also be effective. Can metadynamics help overcome many of the issues inherently present within stochastic gradient descent?

Flow Matching on a Tight Computational Budget - 2026 -

- In conjunction with the flow matching with metadynamics project, I needed a comparative baseline for training flow matching models from scratch. As I don't have organisational resources, I developed the code necessary to train flow matching model from scratch using consumer hardware

A Mathematically Designed and Fabricated Irish Flute - 2024 -

- I obtained access to a lathe, milling machine, and 3D printers. I taught myself precision additive and subtractive manufacturing, as well as design for manufacturing. Combined with my skills in music and encouraged by other folk musicians, I calculated, designed and precision fabricated a series of traditional Irish flutes out of aluminium. These flutes were tested by professional musicians at the Warwick folk festival, and discovered to be comparable to flutes made by professional flutemakers.

Personal ML PyTorch Prototyping Framework - 2019 -

- After years of working with Keras and Tensorflow, I grew sick of how clunky they were. I loved PyTorch, but wanted the abstraction level in Keras. So, I developed a framework called "Lighter" which abstracted training into flexible component hooks. However, I discovered that someone else also had this idea independently. Their idea became the then maturing PyTorch Lightning Framework. So, I abandoned my framework and contributed my work to Lightning. They were even kind enough to send me some merch in the mail!

InfoGAN in PyTorch - 2017 -

- The InfoGAN model was deeply curious to me, as it was one of the early models which seemed to be able to learn labels basically completely unsupervised. So I implemented and played with it myself

Neural Turing Machine in Pytorch - 2017 -

- LSTMs were the cool thing back in 2017, so I was very curious about neural Turing machines

Neural Network Framework in CUDA C - 2015 -

- This was my first big ML project. I was 16 at the time, and this was before the days of Tensorflow and PyTorch. Theano and Keras existed, but they were not well known. So I built my own neural networks framework using only barebones CUDA C. This framework was successful enough to result in its incorporation into the in house ML framework at Leap Motion after I was hired by them

EDUCATION

University Of Warwick, Coventry, UK - *Mathematics of Systems PhD*

September 2022 - October 2026

Leveraging simulations and machine learning to predict the blood brain barrier permeability to drug-like molecules

University Of Warwick, Coventry, UK - *Mathematics of Systems MSc*

September 2021 - August 2022

Distinction

University Of Warwick, Coventry, UK - *Mathematics and Statistics BSc*

September 2017 - June 2020

First Class Honours

OTHER INTERESTS

Folk Violin, Irish Flute, Irish Flute Making , Taekwondo (2nd Degree Black Belt), Hiking, Figure Skating