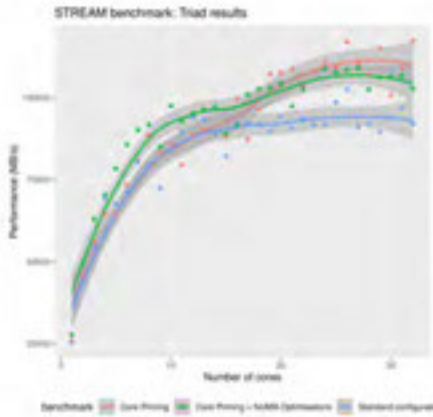


Strategy

General Strategy

- **Profile cluster** with **microbenchmarks** (OSU/STREAM) to understand hardware. Identify and workaround bottlenecks
- Assign **two people** to **each application**
- Test **several compilers** and **flags**
- Use **Intel toolchain** to match CPUs, with vendor **MPI** implementation vs OpenMPI
- **Parameter sweeping**
- **Kernel tuning** for maximal performance
- Further **tuning**, NUMA bindings, CPU affinity, etc
- **Optimise SU usage**, practice on training machine, JetStream2 for production runs

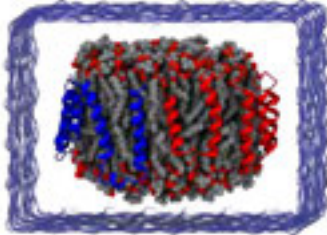


HPL

- Use heuristics to find best **parameter configuration**
- Incrementally increase nodes to ensure **strong scaling**
- Utilise full memory to **maximise compute intensity**

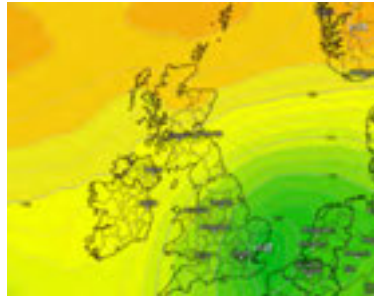
NAMD

- **Compare** x86 optimised binary vs built-from-source
- **CPUs vs GPU**: Experiment to find best performing hardware
- Tweak parameters to balance **speed** vs **accuracy**



ICON

- OpenMP vs OpenMPI - Investigate optimal **thread vs rank split**
- Tune NFS for maximum **I/O throughput**
- **Visualise output** for better scientific understanding



MLPerf

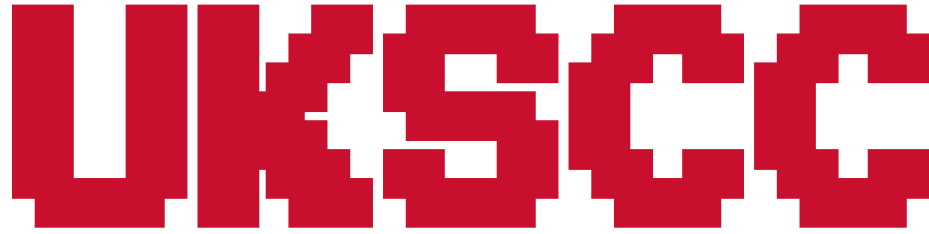
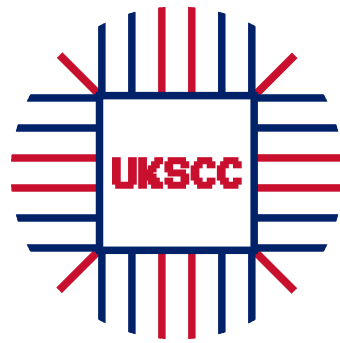
- Use the **latest ML framework** in Python
- Harness **GPUs** for ML performance
- Profile with **nvprof/nsys** for **bottleneck** analysis
- Adjust batch sizes, learning rates etc

Mystery Application

Apply general strategy, and **research** extensively during the homework stage

Running our practice scripts for NAMD, ICON, and MLPerf during the competition

to allows **focus** on the hidden application



Jane Manning, Ethan Ray, Alex Do, Sam Ezeh, Orry Gooberman. Toby Davis

Advisor: Joseph Moore



About Us

We are **UKSCC**, the first team from the UK who have recruited from universities throughout the country. We have 12 total members, with 6 participating in this competition. Our team consists of members from the universities **Bristol**, **Durham**, **Exeter** and **Warwick**. Our ambition is to **win** the competition this year, and return as competitors in next year's SC competition! Within the team we represent multiple different departments, including **Mathematics**, **Computer Science** and **Physics**. This diversity contributes to a large breadth of team knowledge that we will utilise to achieve the **strongest results** in each application. Due to our large pool of applicants from across the whole of the UK, we have an additionally large diversity of backgrounds within the team, with members of **White-British**, **Asian**, **Black-African**, and **White-Other** descent. We also have a mixture of members very **experienced** in HPC competitions, and those **completely new**. Our member selection process involved targeted outreach to universities, including specific societies such as Women in Tech, with the aim to reach underrepresented groups in computer science. Our members submitted an application, and were assessed blindly on merit and performance in HPC practice assignments. This created a **very strong** team, with diverse skills that make us a prime candidate for the winning team!



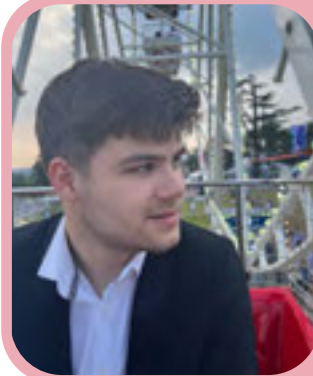
Name: **Jane Manning**
Course: **Mathematics and Physics at Durham**
HPC Experience: **CIUK23 and IndySCC23**
Interest: **Swimming**



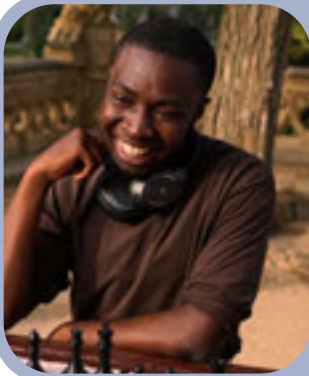
Name: **Alex Do**
Course: **Computer Science at Univeristy of Warwick**
HPC Experience: **New**
Interest: **Piano**



Name: **Orry Gooberman**
Course: **Computer Science at Durham**
HPC Experience: **CIUK22 and ISC23**
Interest: **Theatre**



Name: **Ethan Ray**
Course: **Computer Science and Maths at Exeter**
HPC Experience: **New**
Interest: **Bouldering**

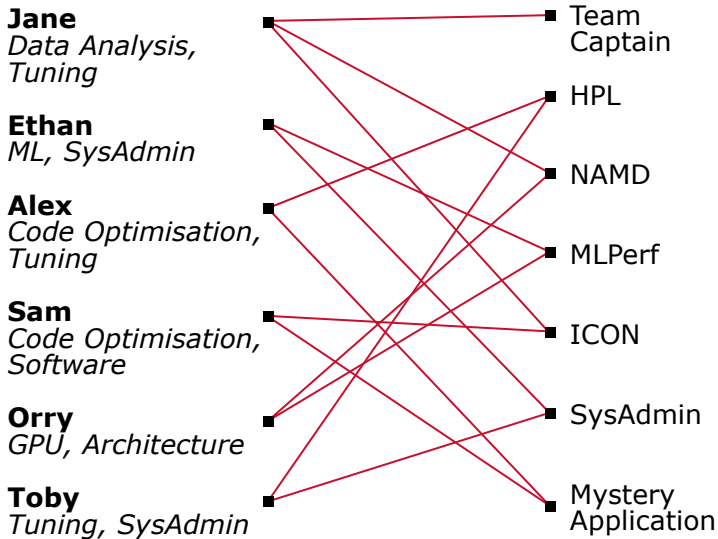


Name: **Sam Ezeh**
Course: **Computer Science at Durham**
HPC Experience: **ISC23, IndySCC23, CIUK23**
Interest: **Chess**



Name: **Toby Davis**
Course: **Computer Science at Durham**
HPC Experience: **New**
Interest: **Mountain Biking**

Distribution of Skills



Infrastructure and Software Setup

JetStream2 Software

- Provisioned with **Ansible** scripts for **fast, repeatable, and scalable** setup
- Optimise **Kernel Parameters** for Rocky 9.4 to achieve **best performance** possible
- Resource management by **Slurm** for **efficient parallel** work
- Environment **modules system** to allow several versions of **compilers** and **libraries**
- User accounts with **sudo** access to **organise workspaces**
- NFS via Gluster Storage Management to **maximise storage** utilisation
- GitHub** repository to hold **record** of scripts and documentation to **maximise** knowledge

HPE Cluster

Sponsored by HPE

- Login Node → Training Team on Similar Hardware
- 2x AMD CPU, 2x A100 40 GB → Practice Applications on HPE Cluster
- 2x AMD CPU, 2x A100 40 GB → Write Portable Scripts
- 2x AMD CPU, 2x A100 80 GB → Production Runs on JetStream2
- 2x AMD CPU, 2x A100 80 GB → Production Runs on JetStream2