

# Scientific Software at Scale: Pawsey Supercomputing Centre Perspective

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## ABSTRACT

The world's fastest supercomputers can now perform 200,000 trillion calculations per second. Software that can get the best out of such hardware is constantly being updated and in need of optimisation. In this talk we will present and discuss collaboration models and outcomes of recent scientific software optimization initiatives led by the Pawsey Supercomputing Centre. Within the last few years, the Pawsey Centre has organised national level hackathon events and opened calls for uptake projects addressed to both industry and research organisations. Most of the projects launched during those initiatives were related to optimisation of workflows, parallelization of existing scientific codes and porting to novel architectures, especially GPUs.

## GPU HACKATHONS

In 2019, the Pawsey Supercomputing Centre hosted a second regional GPU Hackathon in Perth, in collaboration with Oak Ridge National Laboratories (ORNL) and NVIDIA. The event is part of the GPU Hackathon series coordinated by Oak Ridge (<https://www.olcf.ornl.gov/for-users/training/gpu-hackathons/>) and invites participants from across Australasia and SE-Asia. A GPU hackathon is a 5-day coding event in which teams of developers port their applications to run on GPUs, or optimize their applications. Each team consists of three or more developers who are intimately familiar with (some part of) their application, and who work alongside two mentors with GPU programming expertise. The mentors come from universities, national laboratories, supercomputing centres, government institutions, and vendors. There were 5 teams participating in this year's GPU Hackathon: 4 research teams and 1 team from industry organisation. The outcomes of the event will be discussed during the talk and include some outstanding results with speedups ranging from 10 to 1000x compared to initial CPU versions of the codes. We will also discuss future plans to organize similar events to address our user community demands.

## PAWSEY UPTAKE PROJECTS

The Pawsey Supercomputing Centre conducts an annual Uptake Project call, in which successful applicants were provided with approximately 3 months of 0.25 FTE effort from a Pawsey Staff member. These projects provide an opportunity to significantly improve the quality of projects making use of Pawsey facilities. In 2018, there were 13 successful outcomes, including the engagement of new groups to start working with Pawsey, establishing new workflows, and speeding up processing by orders of magnitude. Selected projects will be presented in this talk. As a result of an appraisal of the 2018 Uptake round, several improvements have been made to the process which will also be discussed in the presentation.