Evaluating HPC Architectures for Scientific Computing: Performance, Scalability, and Energy Efficiency

The increasing demands of scientific simulations, big data processing, and artificial intelligence are driving the development of more efficient and powerful CPUs and accelerators. In this rapidly evolving landscape, understanding how scientific applications perform on emerging computing platforms is crucial. Evaluating how legacy codes adapt to novel architectures helps maximise resource utilisation and informs co-design strategies to optimise performance.
In this work, we assess the execution efficiency of widely used scientific codes in high-energy physics, fluid dynamics, material science, and plasma physics across different HPC architectures. We analyse execution time, scalability, and architectural features such as cache hierarchy, vectorisation, and memory bandwidth, while also considering power consumption as a key factor in performance trade-offs.
Our findings offer practical insights for developers, aiding them in selecting the most suitable architecture for their workloads and optimising applications through architecture-aware design strategies.