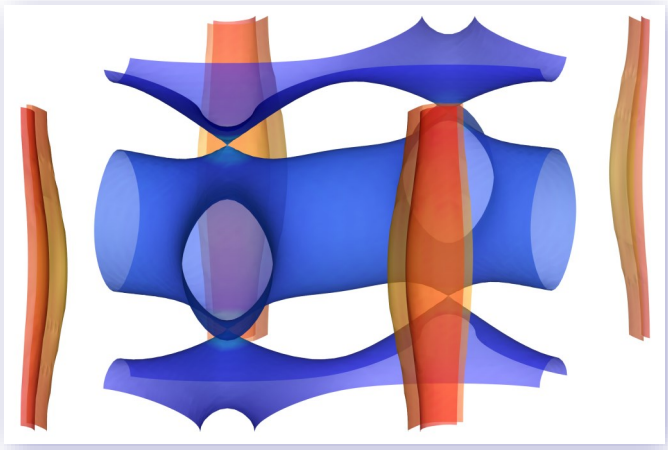
Performance Optimisation and Productivity

HPC Best Practices for Research and Education

Collaboration with POP to achieve academic excellence

- Performance optimisation for parallel research software, allowing better usage of universities' resources and creating capacity for solving more complex problems
- Learning materials and training workshops suitable for MSc level, Ph.D students and Postgraduate researchers.

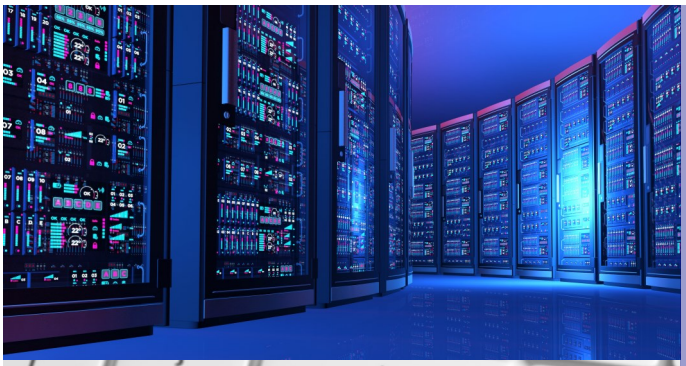


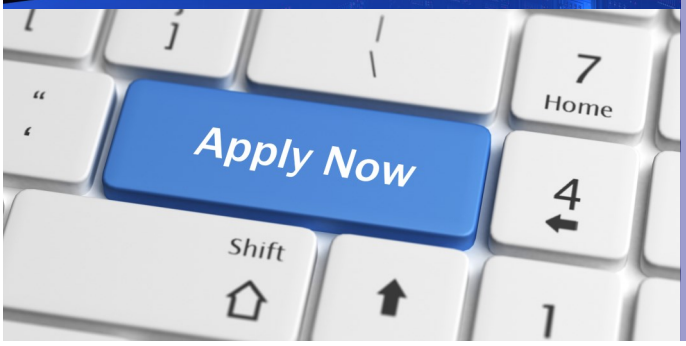
EPW, University of Oxford

POP achieved 10-fold scalability improvement for EPW (Electron-Phonon Coupling using Wannier interpolation), a materials science code developed by researchers at the University of Oxford. Important optimisations included:

- Load imbalance issues were addressed by choosing a finer grain configuration
- Specialized routines were written for one part of the simulation to avoid unnecessary calculations
- Vector summation operations were optimised
- File I/O was optimised, bringing down seven hours of file writing to under one minute.

Your parallel code: better





A Centre of Excellence promoting best practice in parallel programming

- Providing FREE services giving a precise understanding of application performance and system behaviour
- Advice and support on how to refactor code in the most productive way
- Available for EU academic and industrial codes and users

HPC facilities are a major capital investment and often run close to capacity. Improving the efficiency of application software running on these facilities either speeds up time to solution or allows for larger, more challenging problems to be solved. The Performance Optimisation and Productivity (POP) Centre of Excellence exists to help you identify how your software can be improved, free of charge.

Funded by the EU under the Horizon 2020 Research and Innovation Programme, POP puts the world-class HPC expertise of eight commercial and academic partners at your disposal. POP has the tools and expertise to analyse all aspects of performance from single processor efficiency to the scalability of large parallel codes. We work with programs written in most languages and parallel paradigms, including MPI, OpenMP, CUDA, OpenCL and OpenACC.

Our analysis will identify issues such as memory bottlenecks, communication inefficiencies and load imbalances. This allows for a better understanding of program efficiency and the identification of target kernels for code refactoring. We can work on these computational kernels and advise how to roll out improvements to your whole application. As well as reducing run-times, greater efficiency can also lead to reduced power consumption or cloud computing costs. In the first phase of POP we investigated thirty-four codes used by a range of commercial organisations and achieved an average performance improvement over the whole application of 2.25×, i.e. on average we more than halved the time to solution.

Our experience shows that it is often difficult to build a quantitative picture of HPC application behavior. One of the strengths of POP is our set of Metrics. They provide a standard, objective way to characterise different aspects of the performance of parallel codes. These simple measures, the performance data and recommendations are presented to you in a POP Performance Assessment report. This could be followed up by further work, again free to the user, to demonstrate the improvements that those recommendations would make.

Visit the POP Website for learning materials, our blog, and details of how to sign up for our newsletter and webinar programme.

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