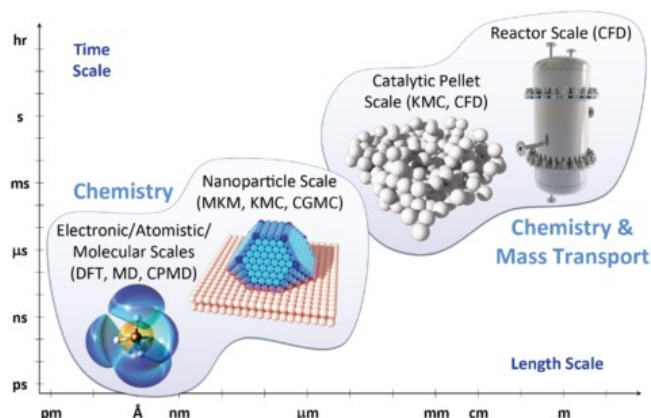




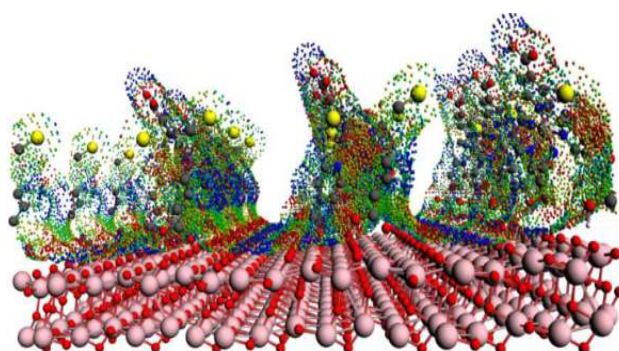
# Performance Optimisation and Productivity



## HPC Performance Optimisation for Materials Science

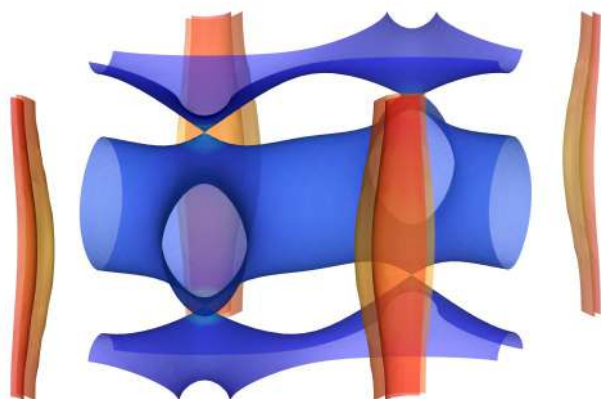
### 10-times Scalability improvement for DFT code

EPW is a materials science DFT code distributed in the Quantum ESPRESSO suite. Developers from the University of Oxford requested a POP performance audit of an unreleased version of the code that was still in development. It was tested with a GaN polar wurtzite crystal dataset on the ARCHER Cray XC30 supercomputer.

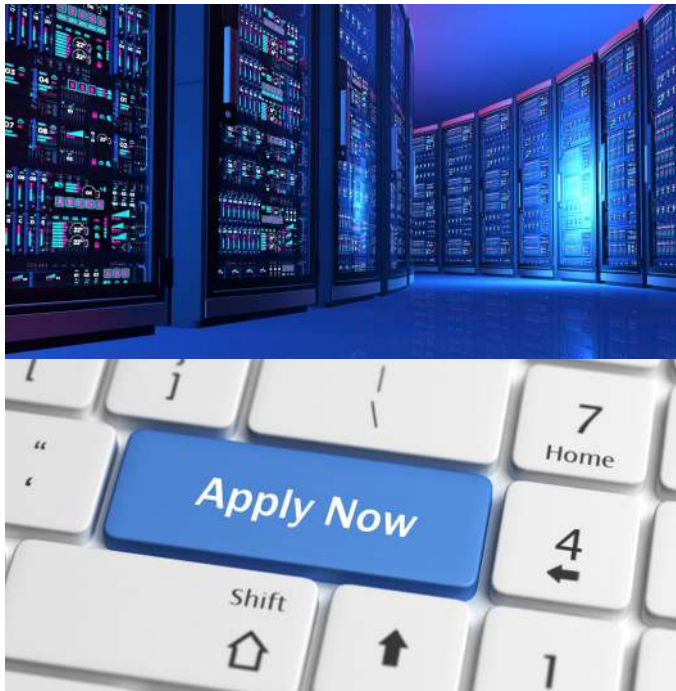


### Performance Improved: SCM's Amsterdam Modeling Suite (AMS)

POP identified a matrix multiplication subroutine which was underperforming. Changes included overlapping computation with communication, improved use of BLAS, and reorganising the algorithm to reduce the amount of data communicated via MPI. The optimised subroutine showed four times speed up over the original code.



**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 2.25x, 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.**

[www.pop-coe.eu](http://www.pop-coe.eu)

✉ [pop@bsc.es](mailto:pop@bsc.es)

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