

Performance Optimisation and **Productivity**

A Centre of Excellence in HPC



POP Newsletter 22 – Issue June 2022

Welcome to the 22nd newsletter from the EU <u>POP</u> Centre of Excellence.

The POP service ended on the 31st May but we hope to return with a third round of funding in a few months' time. In the meantime, please enjoy our newsletter content. Why not catch up on our two latest webinars, "Lessons learned from running an EU Code Optimisation Centre of Excellence" and "Resources for Co-Design" and then read our informative technical blogs on the use of profiling tools? Following that, find out about the recent events we have contributed to and where you can learn more in our forthcoming performance tuning workshops.

If you would like to contribute technical content for this newsletter on the topic of parallel performance profiling, please contact us at <u>pop@bsc.es</u>.

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For past editions of the newsletter, see the POP newsletter web page.

The Future of the POP Service

Sadly, the POP service came to the end of its current round of funding on 31st May, after a great three and a half years of parallel code profiling and optimisation. We hope to continue this valuable work with a third round of EU funding. We will keep you informed of any news!

POP Webinars

Upcoming Event: 25th POP Webinar - Six and a half years of POP CoE: What Remains?

Join us on June 14, 2022 - register here.

The EU Performance Optimisation and Productivity Centre of Excellence in HPC (POP CoE) operated from October 2015 to May 2022. In its lifetime, it provided over 400 Performance Assessments or Proof-of-Concept services free of charge to many academic and research organisations, SMEs, ISVs, and companies in Europe. The services were based on the successful POP Performance Metrics and Methodology developed in the project. It also organized dozens of training courses on performance analysis methods and tools for HPC applications, developed online training modules, and ran a very successful series of webinars. Finally, it developed a "Resources for Co-design" website, which offers a resource for application developers, performance analysts and system designers (hardware and software) to understand the sort of problems they can encounter when executing on HPC systems.

In this final webinar, project coordinator Jesús Labarta from BSC gives an overview of the achievements of the project, discusses its impact, and provides lessons learned after running the POP CoE for six and a half years.

Register here.

Last Event: 24th POP Webinar - Resources for Co-Design

<u>Resources for co-design</u> is a section within the POP website which gathers together a set of typical behavioural patterns seen in HPC codes, potentially resulting in some kind of performance degradation, that POP has identified in our analyses of user applications. For each of these patterns, the site links to the corresponding best-practice(s) that address their performance issues and, in many cases, also provides downloadable benchmarks to allow interested parties to compare the behaviour before and after applying a given best-practice.

In this 30-minute webinar, Xavier Teruel of BSC presented the main motivation behind the development of the site and then explained how to navigate through the different resources for co-design that have so far been created. The recording and slides can be found <u>here</u>.

Browse the full list and catch up on all our previous webinars here.

Technical Blogs

Profiling and Tracing of Python Code with Score-P

The parallel performance and instrumentation framework Score-P only supports Fortran and C/C++ applications by default. However, with the freely available Score-P Python module, it supports Python code as well.

Find out more in this <u>blog post</u>.

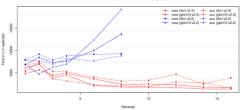
HPC.NRW Tool Talks

HPC.NRW is the competence network for High-Performance Computing in North Rhine-Westphalia, the German state in which POP partners Jülich and RWTH Aachen are both located. Relevant presentations from the HPC.NRW Tool Talk series have been made available to POP users via a series of blog posts. The recordings, slides and any example codes are all included. Specifically, there is

- <u>Application Profiling with Score-P and Cube</u>
- Automated Trace-based Performance Analysis with Score-P & Scalasca
- Lightweight Profiling and Code Quality Assessment with MAQAO

POP helps speedup Genome-Wide Scans with population-specific covariables

A recent POP assessment for the <u>BayPass</u> code gave Mathieu Gautier, the code developer, valuable insight into the cause of low IPC (instructions per cycle), allowing a new version of BayPass with significantly improved parallel scaling, e.g. over 10 times speedup relative to the original version.



Find out more <u>here</u>.

ABINIT Readiness for Exascale Assessed in Campaign for NOMAD CoE

<u>ABINIT</u> is a popular open-source materials science software suite to calculate observable properties of materials, starting from quantum equations of Density Functional Theory (DFT). The Novel Materials Discovery Centre of Excellence <u>NOMAD</u> is readying ABINIT and three other codes as flagships for imminent exascale computer systems, and POP has been analysing them in its periodic assessment campaigns for HPC CoEs.

More details about the POP assessments for ABINIT can be found here.

Recent POP Events

POP Performance Analysis Methodology Workshop

On 15th December 2021, POP delivered its popular **Performance Analysis Methodology Workshop**, held online and organised in collaboration with the <u>Computer Science Department</u> and <u>Advanced Research Computing</u> at Durham University, <u>DiRAC</u> and the <u>N8 CIR</u>. The workshop gave a comprehensive grounding in the basics of performance analysis for research and simulation codes, and explained the POP metrics for MPI, OpenMP and hybrid codes, as well as trace collection using the <u>Barcelona Supercomputer Center's tracing tools</u> and NAG's <u>PyPOP</u>. It attracted an impressive 49 attendees from the UK's HPC research software engineering community.

The slides and a recording of the presentation can be found here.

Diversifying the HPC Community: 2nd Edition of the HPC Training by Women and Underrepresented Group

Following the success of our <u>first training</u>, POP CoE organized the 2nd series of performance analysis and tuning workshops with all-female trainers. This workshop was held from 17th to 19th May 2022 in collaboration with <u>VI-HPS</u>. Marta Garcia-Gasulla (Barcelona Supercomputing Center) and Radita Liem (RWTH Aachen University) were the main organizers of the workshop..

Read everything about this successful training here.

