



Performance Optimisation and Productivity

A Centre of Excellence in HPC



POP Newsletter 14 – Issue March 2020

Welcome to the 14th newsletter from the EU [POP](#) Centre of Excellence. For new requests, please see the section “Apply for free help with Code Optimisation” at the bottom of this newsletter. In this edition, there are two exciting webinar announcements and articles on HPC parallel performance profiling.

This issue includes:

- POP webinar - Energy Efficient Computing using Dynamic Tuning on Thursday 2 April 2020 2pm BST | 3pm CEST;
- POP webinar - CompBioMed CoE - Addressing Biomedical Challenges with High Performance Computing on Friday 15 May 2020 2pm BST | 3pm CEST;
- 190x strong-scaling speed-up of HemeLB simulation on SuperMUC-NG;
- Tool Time: Profiling Tool Support for GPU Programming;
- Tool Time: Measurement of External Libraries with Score-P;
- POP Out and About – meet POP members face to face at the following events:
 - Teratec 2020 Forum. Ecole Polytechnique, Paris. June 16 - 17, 2020;
 - NAFEMS 2020 UK Conference, Milton Keynes, UK. June 9 - 10, 2020.
- Apply for free help with Code Optimisation;
- The POP Helpdesk.

For information on our services and past editions of the newsletter see the [POP website](#).

POP Webinar - Energy Efficient Computing Using Dynamic Tuning

Thursday 2 April 2020 2pm BST | 3pm CEST

We now live in a world of power-constrained architectures and systems, and power consumption represents a significant cost factor in the overall HPC system economy. For these reasons, researchers, supercomputing centres and major vendors have developed new tools and methodologies to measure and optimise the energy consumption of large-scale high performance system installations. Due to the link between energy consumption, power consumption and execution time of an application, it is important for these tools and the methodologies used to consider all these aspects, empowering the user and the system administrator with the capability of finding the best configuration given different high level objectives.

This webinar focuses on tools designed to improve the energy-efficiency of HPC applications using a methodology of dynamic tuning of HPC applications, developed under the H2020 READEX

project. The READEX methodology has been designed for exploiting the dynamic behaviour of software. At design time, different runtime situations (RTS) are detected and optimised system configurations are determined. RTSs with the same configuration are grouped into scenarios, forming the tuning model. At runtime, the tuning model is used to switch system configurations dynamically. We will present the MERIC tool, that implements the READEX methodology. It supports manual or binary instrumentation of the analysed applications to simplify the analysis.

About the Presenter

Lubomir Riha, Ph.D. is the Head of the Infrastructure Research Lab at IT4Innovations National Supercomputing Center. Previously he was a senior researcher in the Parallel Algorithms Research Lab at IT4Innovations and a research scientist in the High Performance Computing Lab at George Washington University, ECE Department. Currently he is a local principal investigator of the H2020 Center of Excellence, POP.

Click on this [link](#) for registration.

POP Webinar - CompBioMed CoE - Addressing Biomedical Challenges with High Performance Computing

Friday 15 May 2020 2pm BST | 3pm CEST

CompBioMed is a European Commission H2020 funded Centre of Excellence focused on the use and development of computational methods for biomedical applications. Since commencing in 2016, the CompBioMed consortium of academic institutions, supercomputing centres and industrial partners have broken new ground in a diverse range of applications in the domain of computational biomedicine. These have been conducted with a particular interest in the fields of cardiovascular simulation, molecular medicine and neuro-musculoskeletal analysis. Collaborations by members of the consortium have led to studies being conducted on some of the latest supercomputing facilities throughout Europe and America.

In this webinar, we will outline some of CompBioMed's achievements on HPC infrastructure in these fields of computational biomedicine. The consortium's efforts to broaden the capability of HPC use within the biomedical community will also be discussed. Finally, we will highlight the results of previous interactions between the CompBioMed and POP CoEs and possible avenues for future collaboration.

About the Presenter

Jon McCullough is a Post-Doctoral Research Associate working in the Centre for Computational Science at University College London on the CompBioMed project. His research is focused on developing the HemeLB code for simulation of human-scale blood flow in arterial and venous geometries.

Click on this [link](#) for registration.

190x strong-scaling speed-up of HemeLB simulation on SuperMUC-NG

HemeLB is an open-source lattice-Boltzmann code for simulation of large-scale three-dimensional fluid flow in complex sparse geometries such as those found in vascular networks. It is written in C++ using MPI and developed by University College London within the EU H2020 HPC CompBioMed Centre of Excellence as their flagship code.

This [blog](#) describes how the code has achieved a speedup of 190x on the SuperMUC-NG HPC cluster.

Tool Time: Profiling Tool Support for GPU Programming

POP expert Michael Knobloch presented an overview of tool support for programming GPUs in the Modular Supercomputing Architecture (MSA) Seminar at Jülich Supercomputing Centre (JSC) on Dec 3, 2019. GPUs are now widely used in HPC applications for their computational capabilities, and getting the best performance requires GPU code to be profiled and subsequently optimised. During the talk, Michael presented the table below, which shows profiling tool support for the different GPU runtime systems. OMPT is the OpenMP tools interface.

Tool	CUDA	OpenACC	OMPT	OpenCL
Score-P	✓	✓	**	✓
NVIDIA Tools	✓	✓	✗	✗
Perf. Reports	✓	*	✗	✗
TAU	✓	✓	**	✓
HPCToolkit	✓	✗	**	✗
Extræe	✓	✗	✗	✓

* = Indirect support via CUDA ([Nvidia](#) only)

** = Prototype with non-public OMP(T) runtime

The blog, with a link to the full presentation, can be found [here](#).

Tool Time: Measurement of External Libraries with Score-P

Very often scientific applications use third-party libraries, e.g. MKL, FFTW, PETSc, etc. Such libraries are the building blocks of applications and often lead to better performance due to being highly optimised. We usually consider these libraries as a black box and assume that the implementation is good enough for the developer's needs. However, applications can still suffer from performance issues when using third-party libraries, which requires performance profiling to identify the causes. Score-P is one profiling tool that can be used to identify performance issues. The default behaviour of Score-P is to ignore third-party libraries calls, simply showing it as application execution, which limits the usefulness of the reports in the Cube GUI. However, Score-P can be configured to show detailed performance metrics of third-party library calls to help the developer identify exact causes of performance issues.

This [blog](#) shows how to configure Score-P to profile third-party library routines.

POP Out and About – meet POP members face to face at the following events

POP will be attending the following events. If you would like to meet a member of the POP team, please email pop-helpdesk@bsc.es and we will happily arrange a meeting with you.

NAFEMS 2020 - Milton Keynes, UK. June 9 - 10, 2020

The 2020 NAFEMS UK Conference will be covering topics ranging from traditional FEA and CFD, to new and emerging areas including artificial intelligence and machine learning. NAFEMS will be bringing all those involved in analysis and simulation together, from every corner of industry and academia, giving attendees an opportunity to advance their knowledge.

POP will be an exhibitor at the conference and will be giving the talk "Parallel Engineering Codes: Performance Optimisation with POP Methodology".

For more information on the conference, please click [here](#).

TERATEC 2020 Forum - Ecole Polytechnique, Paris. June 16 - 17, 2020

The TERATEC Forum is a major event in France that brings together international experts in HPC, simulation and big data. It welcomes more than 1,300 attendees, highlighting the technological and industrial dynamism of HPC and the essential role that France plays in this field.

For more information on the conference, please click [here](#).

If you feel that POP should be attending an event please contact us at pop-helpdesk@bsc.es - suggestions are most welcome!

Apply for free help with code optimisation

We offer a range of [free services](#) designed to help EU organisations improve the performance of parallel software. If you are not getting the performance you need from parallel software or would like to review the performance of a parallel code, please apply for help via the short [Service Request Form](#), or [email us](#) to discuss the service further and how it can be beneficial.

These services are funded by the European Union Horizon 2020 research and innovation programme so there is no direct cost to our users.

The POP Helpdesk

Past and present POP users are eligible to use our [email helpdesk \(pop-helpdesk@bsc.es\)](mailto:pop-helpdesk@bsc.es). Please contact our team of experts for help analysing code changes, to discuss your next steps, and to ask questions about your parallel performance optimisation.



<https://pop-coe.eu>



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 676553 and 824080.

