The POP Centre of Excellence - Improving Parallel Codes

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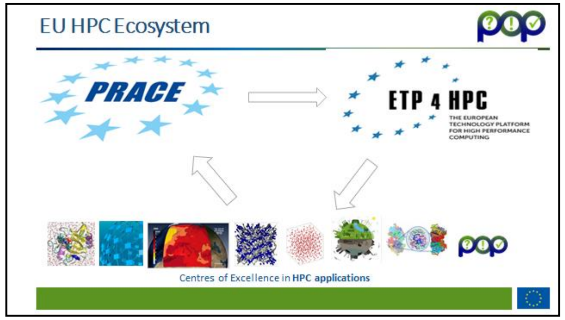
EU H2020 Centre of Excellence (CoE)

1 December 2018 – 30 November 2021

Grant Agreement No 824080

POP CoE

- A **Centre of Excellence**
  - On **Performance Optimisation and Productivity**
  - Promoting **best practices in parallel programming**



EU HPC Ecosystem

PRACE
ETP 4 HPC
THE EUROPEAN TECHNOLOGY PLATFORM FOR HIGH PERFORMANCE COMPUTING

Centres of Excellence in **HPC applications**

- Providing **FREE** Services
  - Precise understanding of application and system behaviour
  - Suggestion/support on how to refactor code in the most productive way
  - Or confirmation that all is good!
  - Approaching 200 services so far.
- Horizontal
  - Transversal across application areas, platforms, scales
- For (EU) **academic AND industrial** codes and users!

POP Team

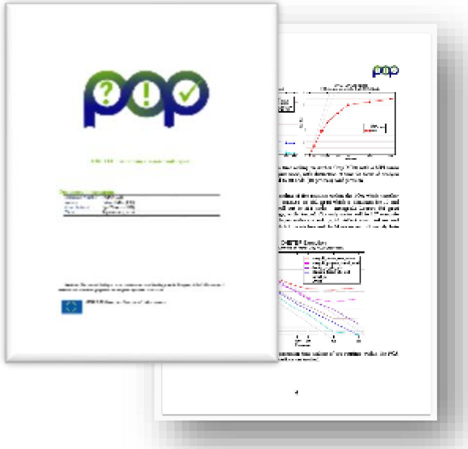
- **Who**
  - BSC, ES
  - HLRS, DE
  - IT4I, CZ
  - JSC, DE
  - NAG, UK
  - RWTH Aachen, DE
  - TERATEC, FR
  - UVSQ, FR
- **A team with**
  - Excellence in performance tools and tuning
  - Excellence in programming models and practices
  - R & D background in real academic and industrial use cases
- **Developing open-source tools**
  - Extrae, Paraver & Dimemas
  - Score-P, Cube & Scalasca
  - MAQAO

Motivation

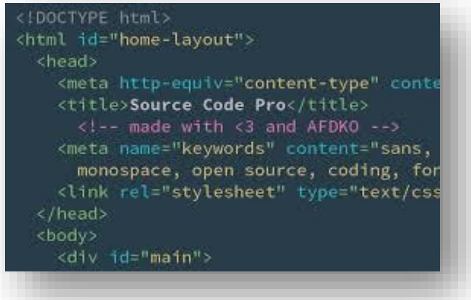
- **Why?**
  - HPC machines and codes getting ever more complex
    - ⇨ Difficult to build quantitative picture of application behaviour
    - ⇨ Often unclear what is best approach to improve performance
  - Important to maximize efficiency (performance, power) of compute intensive applications and productivity of the development efforts
- **What?**
  - Parallel programs, mainly MPI/OpenMP
  - Although also CUDA, OpenCL, OpenACC, Python, …

Services provided by POP

- **Parallel Application Performance Assessment**
  - Identifies performance issues of customer code (at customer site)
  - Possibly restricted to a “region of interest”
  - If needed, identifies the root causes of the issues found and qualifies and quantifies approaches to address them (recommendations)
  - A report is produced
  - Medium effort (1-3 months)



- **Proof-of-Concept**
  - Follow-up service
  - Experiments and mock-up tests for customer codes
  - Kernel extraction, parallelisation, mini-apps experiments to show effect of proposed optimisations
  - Larger effort (3-6 months)

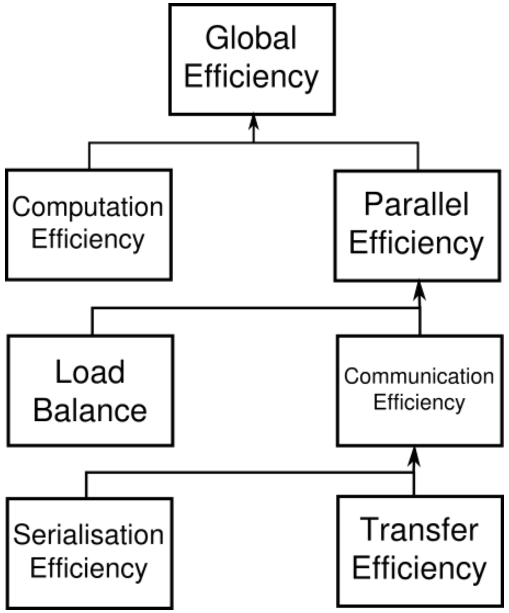


```
<!DOCTYPE html>
<html id="home-layout">
  <head>
    <meta http-equiv="content-type" conte
    <title>Source Code Pro</title>
      <!-- made with <3 and AFDKO -->
    <meta name="keywords" content="sans,
      monospace, open source, coding, for
    <link rel="stylesheet" type="text/css
  </head>
  <body>
    <div id="main">
```

Note: Effort shared between our experts and customer!

POP Metrics

- The following metrics are used in a POP Performance Assessments:
- A numerical measure between 0.0 (bad) and 1.0 (perfect)
- Global Efficiency (GE): GE = PE * CompE
  - Parallel Efficiency (PE): PE = LB * CommE
    - **Load Balance** Efficiency (LB): LB = avg(CT)/max(CT)
    - **Communication** Efficiency (CommE): CommE = SerE * TE
      - Serialization Efficiency (SerE):
        SerE = max (CT / TT on ideal network)
      - Transfer Efficiency (TE): TE = TT on ideal network / TT
  - (Serial) **Computation** Efficiency (CompE)
    - Computed out of IPC Scaling and Instruction Scaling
    - For strong scaling: ideal scaling -> efficiency of 1.0

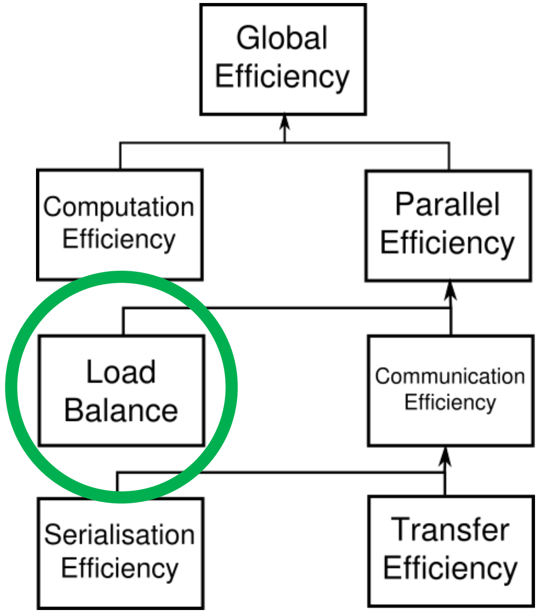


CT = Computational time
TT = Total time

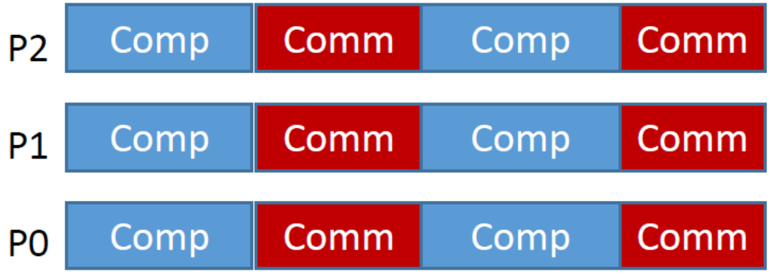
POP Metrics – Parallel Efficiency 1

- Consists of **Load Balance** Efficiency (LB) which reflects how well the distribution of work to threads/processes is done in the application:

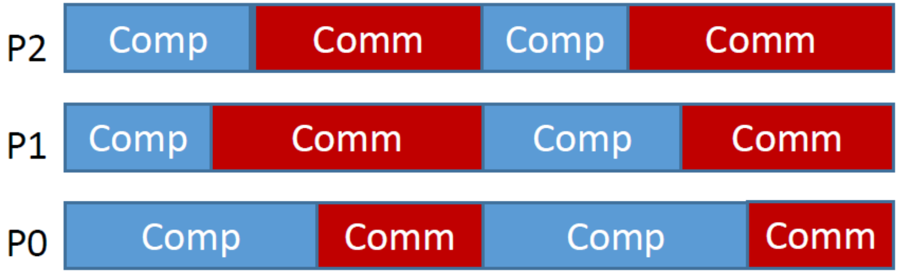
$$LB = \frac{\text{average computational time}}{\text{max computational time}}$$



Example 1: good load balance (LB = 100%)



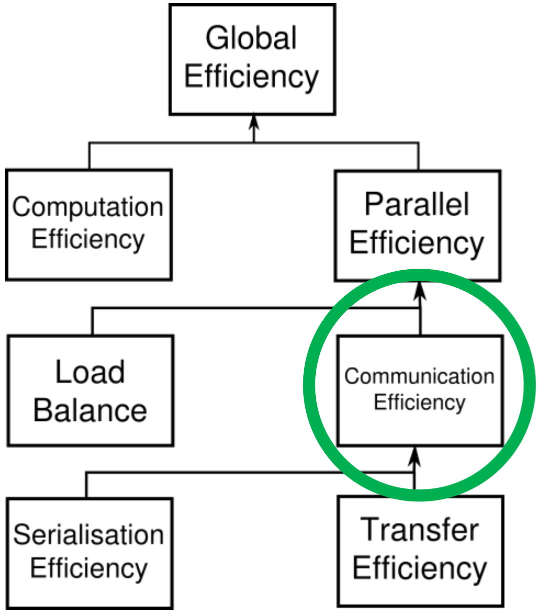
Example 2: bad load balance (LB = 77%)



CT = Computational time
TT = Total time

POP Metrics – Parallel Efficiency 2

- And **Communication Efficiency**: CommE = SerE * TE
  - **Serialization Efficiency** describes loss of efficiency due to dependencies between processes, waiting in MPI, say:
    SerE = max (CT / TT on ideal network)
  - **Transfer Efficiency** describes loss of efficiency due to actual data transfer:
    TE = TT on ideal network / TT



Global Efficiency

Computation Efficiency

Parallel Efficiency

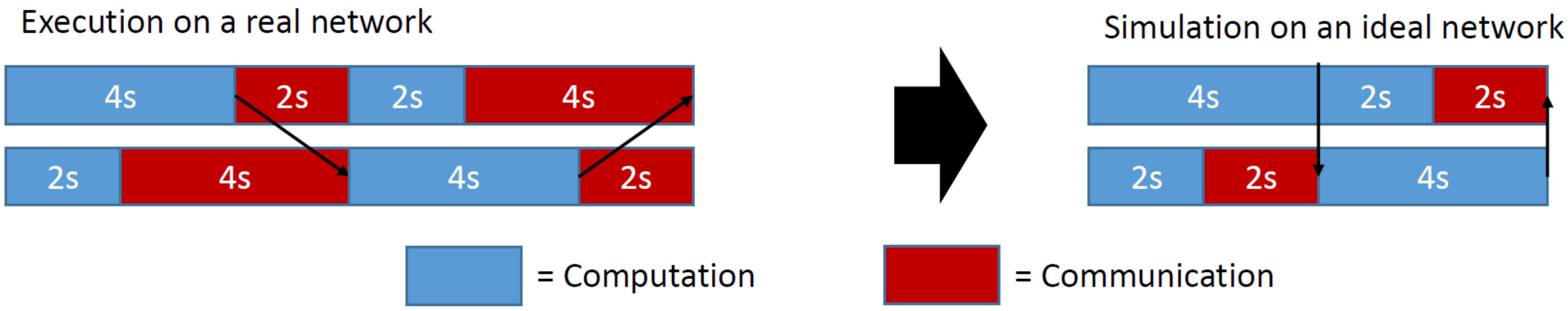
Load Balance

Communication Efficiency

Serialisation Efficiency

Transfer Efficiency

CT = Computational time
TT = Total time

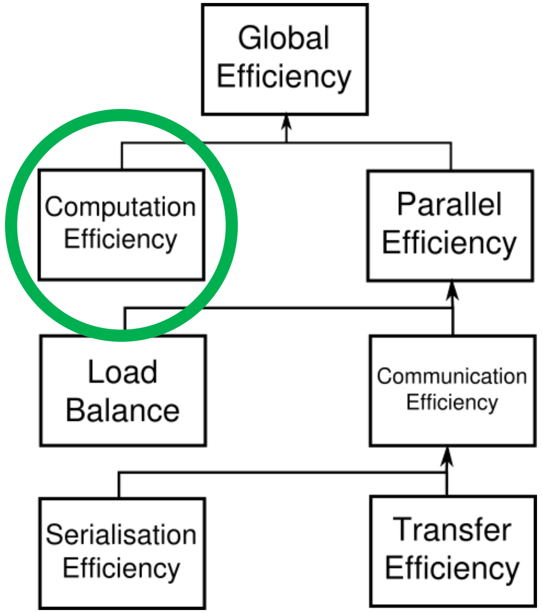


$$\text{SerE} = \frac{6}{8} = 75\%$$

$$\text{TE} = \frac{8}{12} = 66.6\%$$

POP Metrics – Comp. Efficiency

- (Serial) **Computation Efficiency** (CompE)
  - Computed out of IPC Scaling and Instruction Scaling
  - Describes how well the computational load of an application scales with the number of processes.
- **Instruction Scaling** compares the total number of instructions executed for a different number of threads/processes.
- With more processes more instructions may be executed, e.g. some extra computation for the domain decomposition is needed.
- **IPC Scaling** compares how many instructions per cycle are executed for a different number of threads/processes.
- The same number of instructions is computed but the computation takes more time, say. This can happen e.g. due to shared recourses like memory channels.



CT = Computational time
TT = Total time

POP Metrics

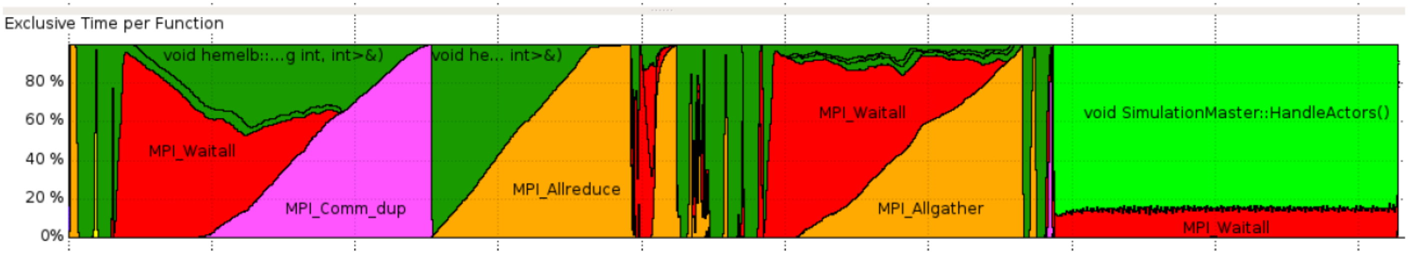
- Simply presented as:

		2	4	8	16
Global efficiency		0.98	0.90	0.78	0.59
X	**Computation Efficiency**	1.00	0.96	0.90	0.76
	Parallel Efficiency	0.98	0.94	0.90	0.85
X	**Load Balance**	0.99	0.97	0.91	0.92
	Communication Efficiency	0.98	0.97	0.98	0.92
X	**Serialization efficiency**	0.99	0.98	0.99	0.94
	Transfer Efficiency	0.99	0.99	0.99	0.98

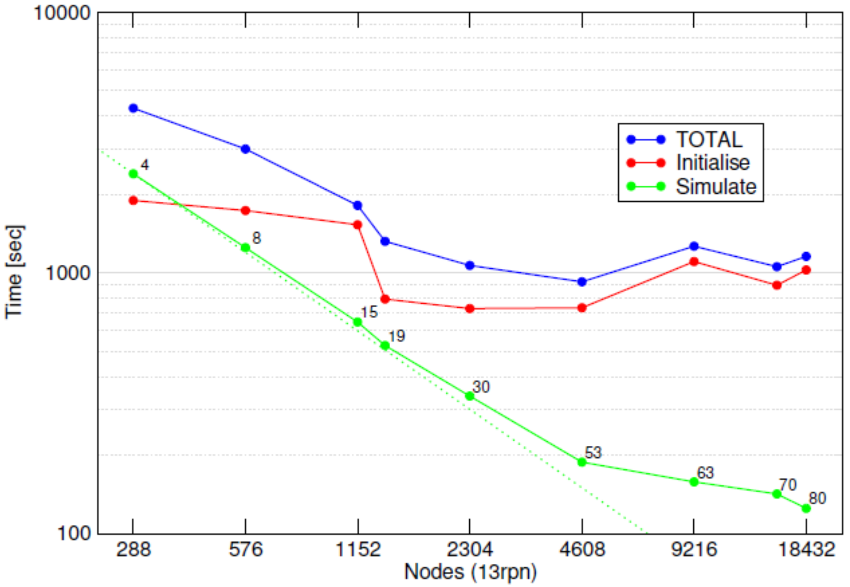
X	**IPC Scaling**	1.00	0.99	0.96	0.84
	Instruction Scaling	1.00	0.97	0.94	0.91

POP and CompBioMed

- POP working with CompBioMed on flagship code HemeLB. (C++ & MPI)
- Analysis helped in development of a new version of HemeLB including a new load-balancing library from E-CAM



- Studies show excellent communication efficiency and strong scaling (up to 239,615 MPI processes Blue Waters Cray XE.)
- Observations also include load balancing affected by one (weak) process per node.
- Would benefit from reduction in memory footprint as some cores unused on node.



See summary and reports

Return on Investment Examples

Application Savings after POP Proof-of-Concept

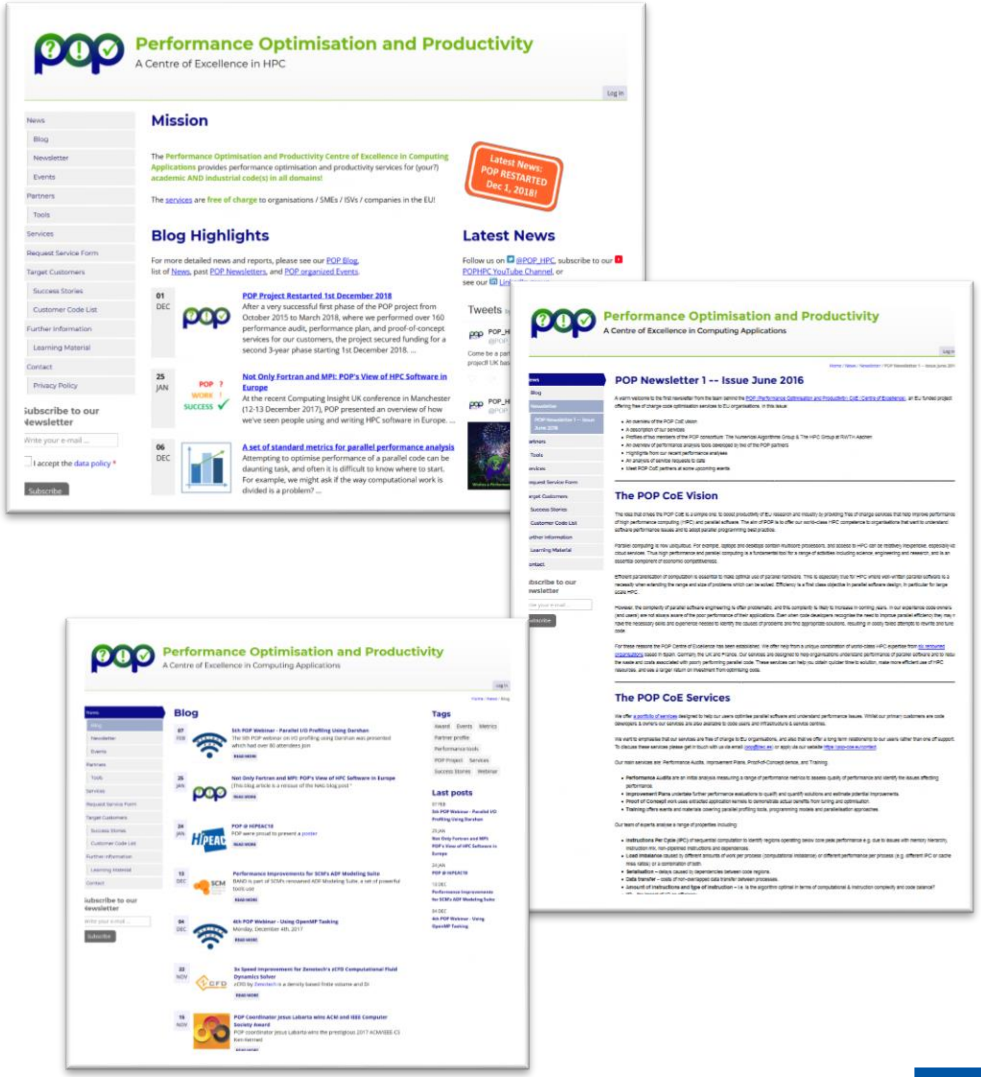
- POP PoC resulted in 72% faster-time-to-solution
- Production runs on ARCHER (UK national academic supercomputer)
- Improved code saves €15.58 per run
- Yearly savings of around €56,000 (from monthly usage data)

Application Savings after POP Performance Assesment

- Cost for customer implementing POP recommendations: €2,000
- Achieved improvement of 62%
- €20,000 yearly operating cost
- Resulted in yearly saving of €12,400 in compute costs ⇨ ROI of 620%

POP Website

- www.pop-coe.eu
- All the information you need to access POP services, and…
- Blogs
- Newsletter: subscribe and archive
- Information on our webinar series, also…



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A Centre of Excellence in HPC

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Mission

The Performance Optimisation and Productivity Centre of Excellence in Computing Applications provides performance optimisation and productivity services for (your?) academic AND industrial code(s) in all domains!

The services are free of charge to organisations / SMEs / ISVs / companies in the EU!

Latest News: POP RESTARTED Dec 1, 2018!

Blog Highlights

For more detailed news and reports, please see our POP Blog, list of News, past POP Newsletters, and POP organized Events.

01 DEC **POP Project Restarted 1st December 2018**
After a very successful first phase of the POP project from October 2015 to March 2018, where we performed over 160 performance audit, performance plan, and proof-of-concept services for our customers, the project secured funding for a second 3-year phase starting 1st December 2018. ...

25 JAN **Not Only Fortran and MPI: POP's View of HPC Software in Europe**
At the recent Computing Insight UK conference in Manchester (12-13 December 2017), POP presented an overview of how we've seen people using and writing HPC software in Europe. ...

06 DEC **A set of standard metrics for parallel performance analysis**
Attempting to optimise performance of a parallel code can be daunting task, and often it is difficult to know where to start. For example, we might ask if the way computational work is divided is a problem? ...

Latest News

Follow us on @POP_HPC, subscribe to our POPHPC YouTube Channel, or see our Lin[illegible]

Tweets

Performance Optimisation and Productivity
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POP Newsletter 1 -- Issue June 2016

A warm welcome to the first newsletter from the team behind the POP (Performance Optimisation and Productivity) CoE (Centre of Excellence), an EU funded project offering free of charge code optimisation services to EU organisations. In this issue:

- An overview of the POP CoE vision
- A description of our services
- Profiles of two members of the POP consortium: The Numerical Algorithms Group & The HPC Group at RWTH Aachen
- An overview of performance analysis tools developed by two of the POP partners
- Highlights from our recent performance analyses
- An analysis of service requests to date
- Meet POP CoE partners at some upcoming events

The POP CoE Vision

[illegible]

The POP CoE Services

[illegible]

- **Performance Audits** [illegible]
- **Improvement Plans** [illegible]
- **Proof of Concept** [illegible]
- **Training** [illegible]

- **Instructions Per Cycle (IPC)** [illegible]
- **Load imbalance** [illegible]
- **Serialisation** [illegible]
- **Data transfer** [illegible]
- **Amount of instructions and type of instruction** [illegible]

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Blog

07 FEB **5th POP Webinar - Parallel I/O Profiling Using Darshan**
The 5th POP webinar on I/O profiling using Darshan was presented which had over 80 attendees join
READ MORE

25 JAN **Not Only Fortran and MPI: POP's View of HPC Software in Europe**
(This blog article is a reissue of the NAG blog post "
READ MORE

24 JAN **POP @ HiPEAC18**
POP were proud to present a poster
READ MORE

13 DEC **Performance Improvements for SCM's ADF Modeling Suite**
BAND is part of SCM's renowned ADF Modeling Suite, a set of powerful tools use
READ MORE

04 DEC **4th POP Webinar - Using OpenMP Tasking**
Monday, December 4th, 2017
READ MORE

22 NOV **3x Speed Improvement for Zenotech's zCFD Computational Fluid Dynamics Solver**
zCFD by Zenotech is a density based finite volume and D
READ MORE

15 NOV **POP Coordinator Jesus Labarta wins ACM and IEEE Computer Society Award**
POP coordinator Jesus Labarta wins the prestigious 2017 ACM/IEEE-CS Ken Kennedy

Tags

Award Events Metrics Partner profile Performance tools POP Project Services Success Stories Webinar

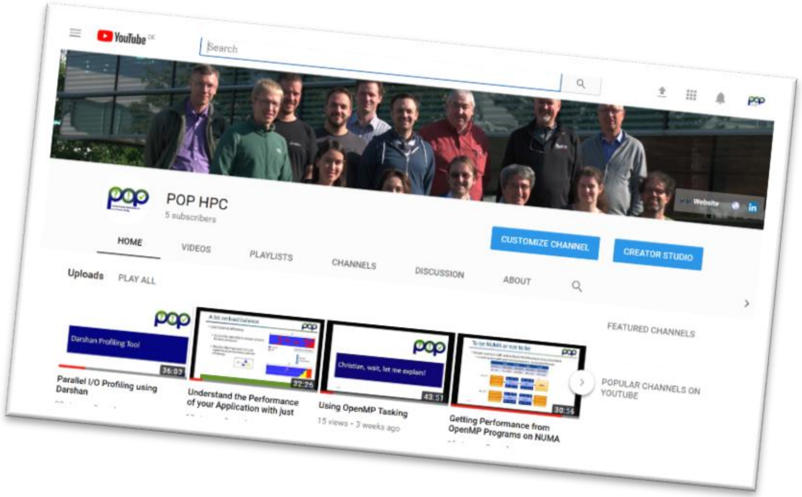
Last posts

07 FEB 5th POP Webinar - Parallel I/O Profiling Using Darshan
25 JAN Not Only Fortran and MPI: POP's View of HPC Software in Europe
24 JAN POP @ HiPEAC18
13 DEC Performance Improvements for SCM's ADF Modeling Suite
04 DEC 4th POP Webinar - Using OpenMP Tasking

YouTube

- See our YouTube Channel

  https://www.youtube.com/pophpc



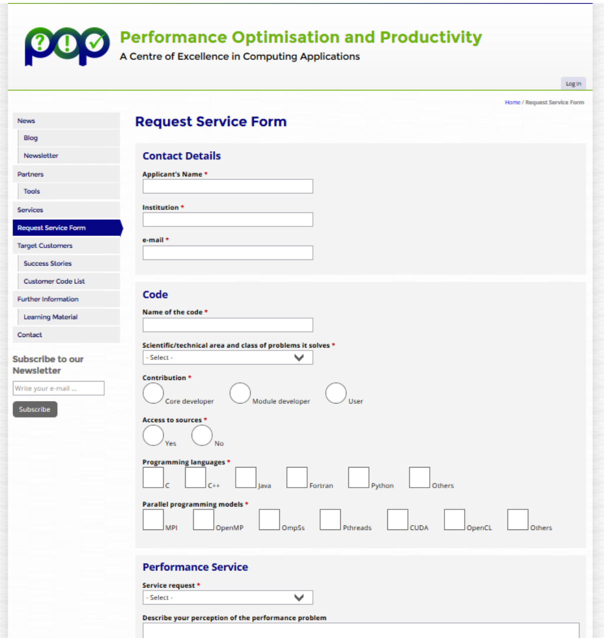
- Recordings available:
  - How to Improve the Performance of Parallel Codes
  - Getting Performance from OpenMP Programs on NUMA Architectures
  - Understand the Performance of your Application with just Three Numbers
  - Using OpenMP Tasking
  - Parallel I/O Profiling Using Darshan
  - The impact of sequential performance on parallel codes
  - Large scale Application Execution Performance Assessment

The POP Process

- **When?**

  POP runs to November 2021

- **How?**
  - Fill in small questionnaire describing application and needs https://pop-coe.eu/request-service-form
  - Questions? Ask pop@bsc.es



Request Service Form

Contact Details

Applicant's Name *

Institution *

e-mail *

Code

Name of the code *

Scientific/technical area and class of problems it solves *

- Select -

Contribution *

○ Core developer ○ Module developer ○ User

Access to sources *

○ Yes ○ No

Programming languages *

□ C □ C++ □ Java □ Fortran □ Python □ Others

Parallel programming models *

□ MPI □ OpenMP □ OmpSs □ Pthreads □ CUDA □ OpenCL □ Others

Performance Service

Service request *

- Select -

Describe your perception of the performance problem

- Install tools on your production machine (local, PRACE, …)
- Collaboratively: Gather data → Analysis → Report

Performance Optimisation and Productivity

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Contact:

https://www.pop-coe.eu

mailto:pop@bsc.es

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NAG is hiring for POP!

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