



On the ROI of Parallel Performance Optimization

Bernd Mohr (Jülich Supercomputing Centre)

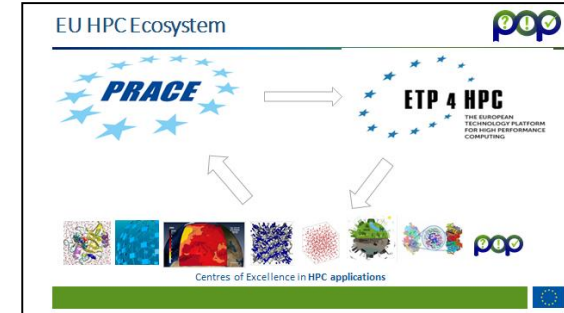
EU H2020 Centre of Excellence (CoE)



1 December 2018 – 30 November 2021

Grant Agreement No 824080

- A **Centre of Excellence**
 - On **Performance Optimisation and Productivity**
 - Promoting **best practices in parallel programming**
- Providing **FREE Services**
 - Precise understanding of application and system behaviour
 - Suggestion/support on how to refactor code in the most productive way
- **Horizontal**
 - Transversal across application areas, platforms, scales
- **For (EU) academic AND industrial codes and users !**



• Who?

- BSC, ES (coordinator)
- HLRS, DE
- IT4I, CZ
- JSC, DE
- NAG, UK
- RWTH Aachen, IT Center, DE
- TERATEC, FR
- UVSQ, FR



A team with

- Excellence in performance tools and tuning
- Excellence in programming models and practices
- Research and development background AND proven commitment in application to real academic and industrial use cases

Why?

- Complexity of machines and codes
 - ⇒ Frequent lack of quantified understanding of actual behaviour
 - ⇒ Not clear most productive direction of code refactoring
- 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, ...

The Process ...



When?

December 2018 – November 2021

How?

- Apply
 - Fill in small questionnaire describing application and needs
<https://pop-coe.eu/request-service-form>
 - Questions? Ask pop@bsc.es
- Selection/assignment process
- Install tools @ your production machine (local, PRACE, ...)
- Interactively: Gather data → Analysis → Report

The screenshot shows the 'Request Service Form' on the POP website. The header includes the POP logo and the text 'Performance Optimisation and Productivity - A Centre of Excellence in Computing Applications'. A sidebar on the left contains links to News, Blog, Newsletter, Partners, Tools, Services, Request Service Form (highlighted), Target Customers, Success Stories, Customer Code List, Further Information, Learning Material, and Contact. Below the sidebar is a 'Subscribe to our Newsletter' section with an email input field and a 'Subscribe' button. The main form area is titled 'Request Service Form' and contains several sections: 'Contact Details' with fields for Applicant's Name, Institution, and e-mail; 'Code' with a field for Name of the code, a dropdown for Scientific/technical area, and radio buttons for Contribution (Core developer, Module developer, User); 'Access to sources' with radio buttons for Yes/No; 'Programming languages' with checkboxes for C, C++, java, Fortran, Python, and Others; 'Parallel programming models' with checkboxes for MPI, OpenMP, OpenSs, Pthreads, CUDA, OpenCL, and Others; 'Performance Service' with a dropdown for Service request; and a text area for 'Describe your perception of the performance problem'.

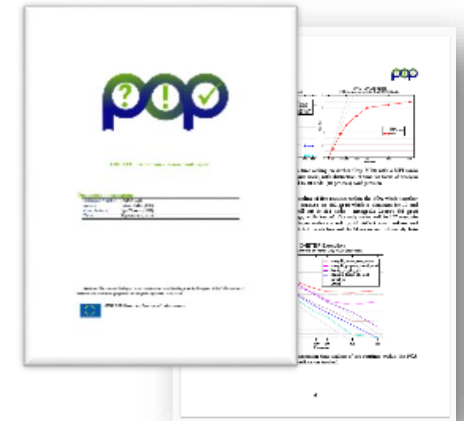


FREE Services provided by the CoE



- **Parallel Application Performance Assessment**

- Primary service
- Identifies performance issues of customer code (at customer site)
- If needed, identifies the root causes of the issues found and qualifies and quantifies approaches to address them (recommendations)
- **Combines former Performance Audit (?) and Plan (!)**
- 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">
```

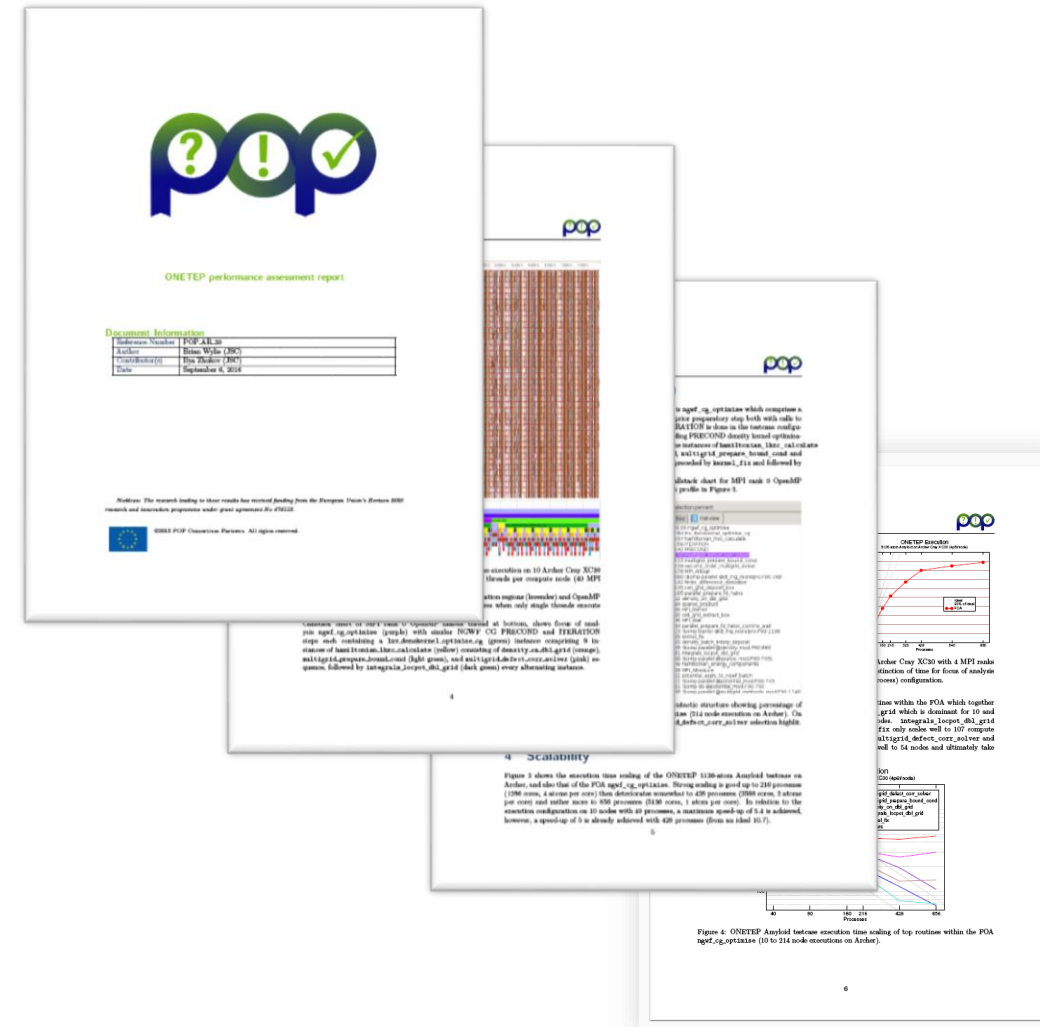
Note: Effort shared between our experts and customer!



Outline of a Typical Audit Report



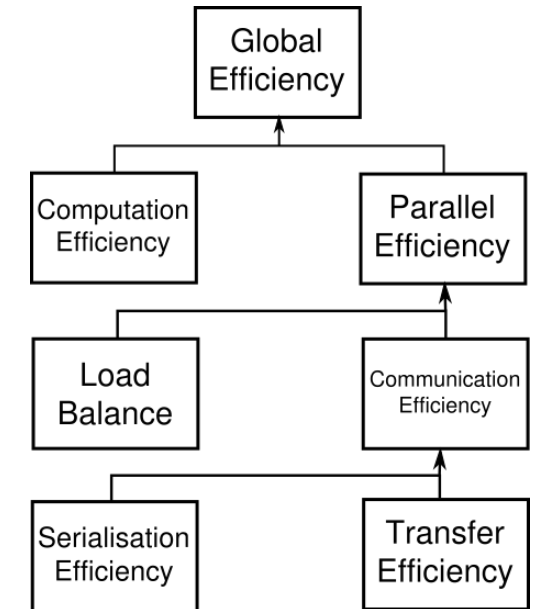
- Application Structure
- (If appropriate) Region of Interest
- Scalability Information
- Application Efficiency
 - E.g. time spent outside MPI
- Load Balance
 - Whether due to internal or external factors
- Serial Performance
 - Identification of poor code quality
- Communications
 - E.g. sensitivity to network performance
- Summary and Recommendations



Efficiencies



- The following metrics are used in a POP Performance Audit:
- 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):
 $SerE = max(CT / TT \text{ on ideal network})$
 - Transfer Efficiency (TE): $TE = TT \text{ on ideal network} / TT$
 - (Serial) **Computation** Efficiency (CompE)
 - Computed out of IPC Scaling and Instruction Scaling
 - For strong scaling: ideal scaling -> efficiency of 1.0
- Details see <https://sharepoint.ecampus.rwth-aachen.de/units/rz/HPC/public/Shared%20Documents/Metrics.pdf>



CT = Computational time
TT = Total time

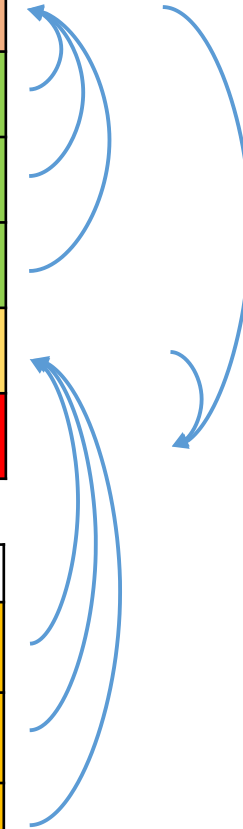


Efficiencies



	2	4	8	16
Parallel Efficiency	0.98	0.94	0.90	0.85
Load Balance	0.99	0.97	0.91	0.92
Serialization efficiency	0.99	0.98	0.99	0.94
Transfer Efficiency	0.99	0.99	0.99	0.98
Computation Efficiency	1.00	0.96	0.87	0.70
Global efficiency	0.98	0.90	0.78	0.59

	2	4	8	16
IPC Scaling Efficiency	1.00	0.99	0.96	0.84
Instruction Scaling Efficiency	1.00	0.97	0.94	0.91
Core frequency efficiency	1.00	0.99	0.96	0.91



- **Install and use already available monitoring and analysis technology**
 - Analysis and predictive capabilities
 - Delivering insight
 - With extreme detail
 - Up to extreme scale
- **Open-source toolsets**
 - Extrae + Paraver
 - Score-P + Cube + Scalasca/TAU/Vampir
 - Dimemas, Extra-P
 - MAQAO
- **Commercial toolsets**
(if available at customer site)
 - Intel tools
 - Cray tools
 - ARM tools

- **Code developers**

- Assessment of detailed actual behaviour
- Suggestion of most productive directions to refactor code

- **Users**

- Assessment of achieved performance in specific production conditions
- Possible improvements modifying environment setup
- Evidence to interact with code provider

- **Infrastructure operators**

- Assessment of achieved performance in production conditions
- Possible improvements from modifying environment setup
- Information for time computer time allocation processes
- Training of support staff

- **Vendors**

- Benchmarking
- Customer support
- System dimensioning/design



Overview of Codes Investigated

Status after 2½ Years (End of Phase1)



Performance Audits and Plans

- 139 completed or reporting to customer
- 13 more in progress

Proof-of-Concept

- 19 completed Proofs of Concept
- 3 more in progress



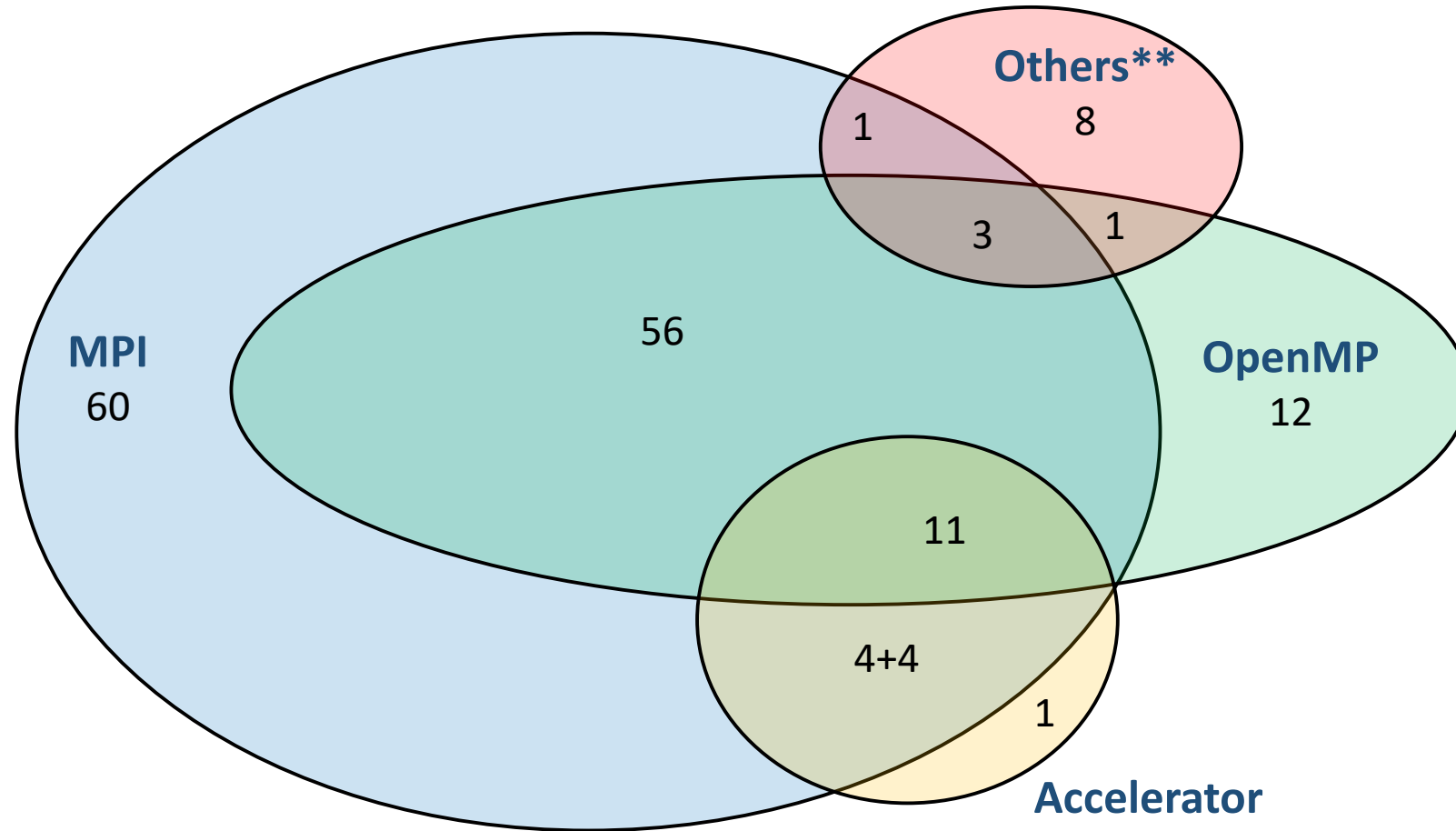
Example POP Users and Their Codes



Area	Codes
Computational Fluid Dynamics	DROPS (RWTH Aachen), Nek5000 (PDC KTH), SOWFA (CENER), ParFlow (FZ-Juelich), FDS (COAC) & others
Electronic Structure Calculations	ADF, BAND, DFTB (SCM), Quantum Espresso (Cineca), FHI-AIMS (University of Barcelona), SIESTA (BSC), ONETEP (University of Warwick)
Earth Sciences	NEMO (BULL), UKCA (University of Cambridge), SHEMAT-Suite (RWTH Aachen), GITM (Cefas) & others
Finite Element Analysis	Ateles, Musubi (University of Siegen) & others
Gyrokinetic Plasma Turbulence	GYSELA (CEA), GS2 (STFC)
Materials Modelling	VAMPIRE (University of York), GraGLeS2D (RWTH Aachen), DPM (University of Luxembourg), QUIP (University of Warwick), FIDIMAG (University of Southampton), GBmolDD (University of Durham), k-Wave (Brno University), EPW (University of Oxford) & others
Neural Networks	OpenNN (Artelnics)



Programming Models Used

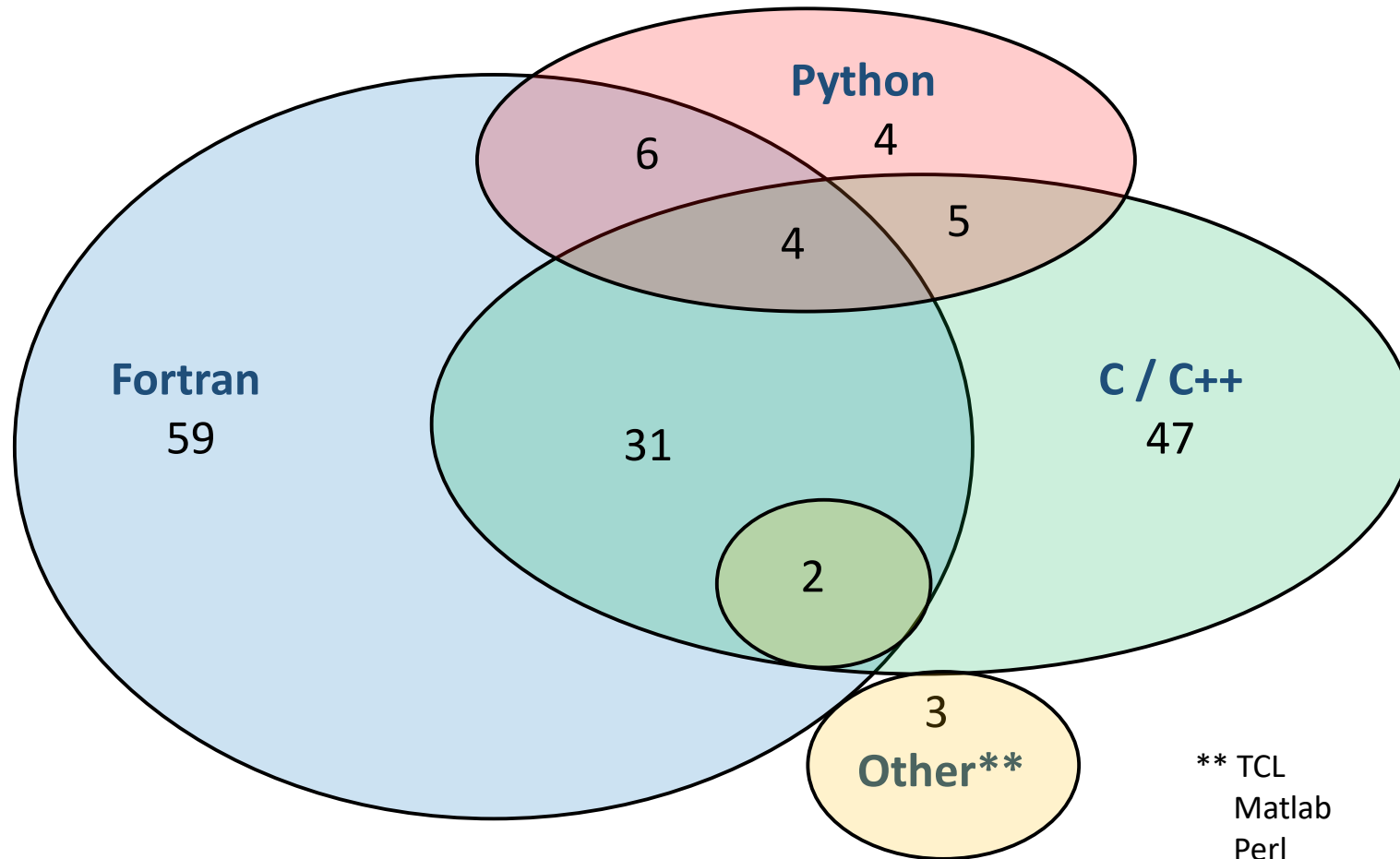


** MAGMA
Celery
TBB
GASPI
C++ threads
MATLAB PT
StarPU
GlobalArrays
Charm++
Fortran Coarray

* Based on data collected for 161 POP Performance Audits



Programming Languages Used

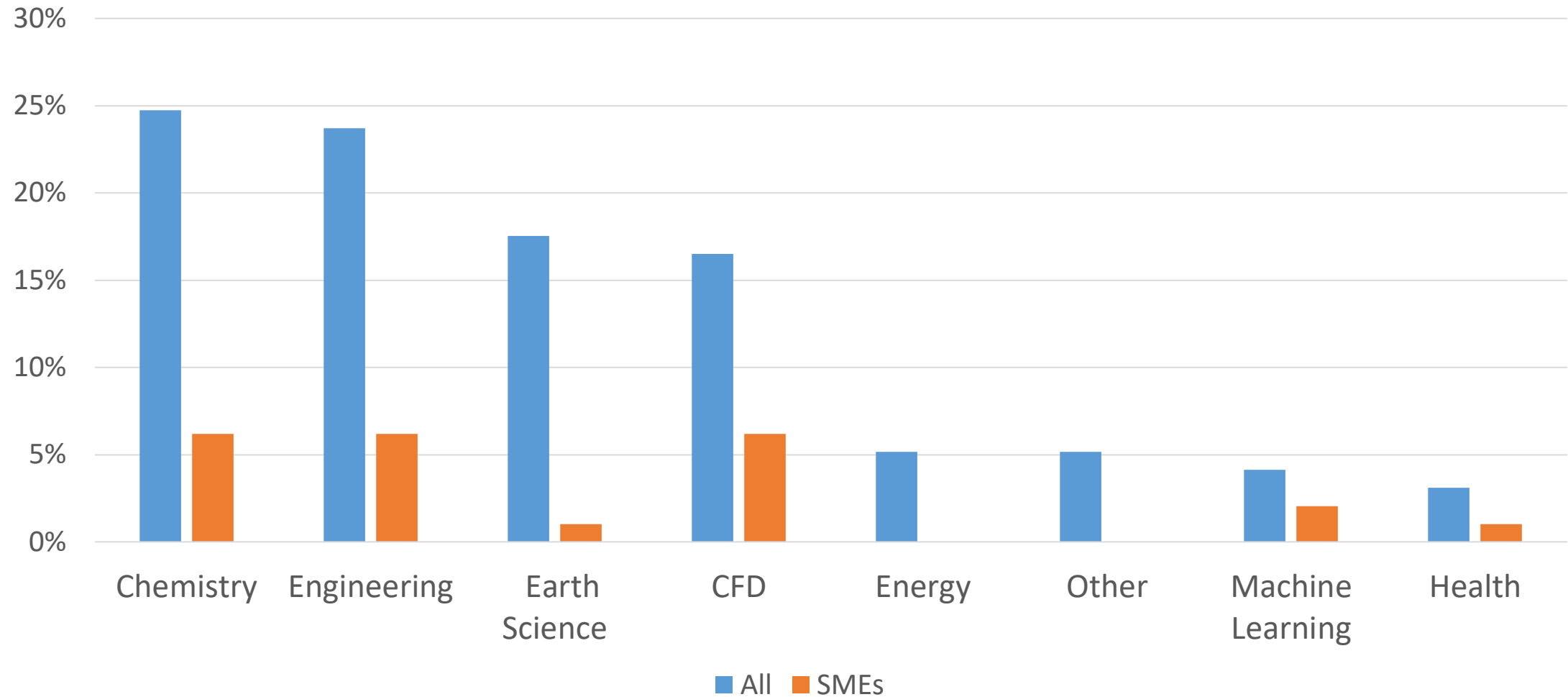


** TCL
Matlab
Perl
Octave
Java

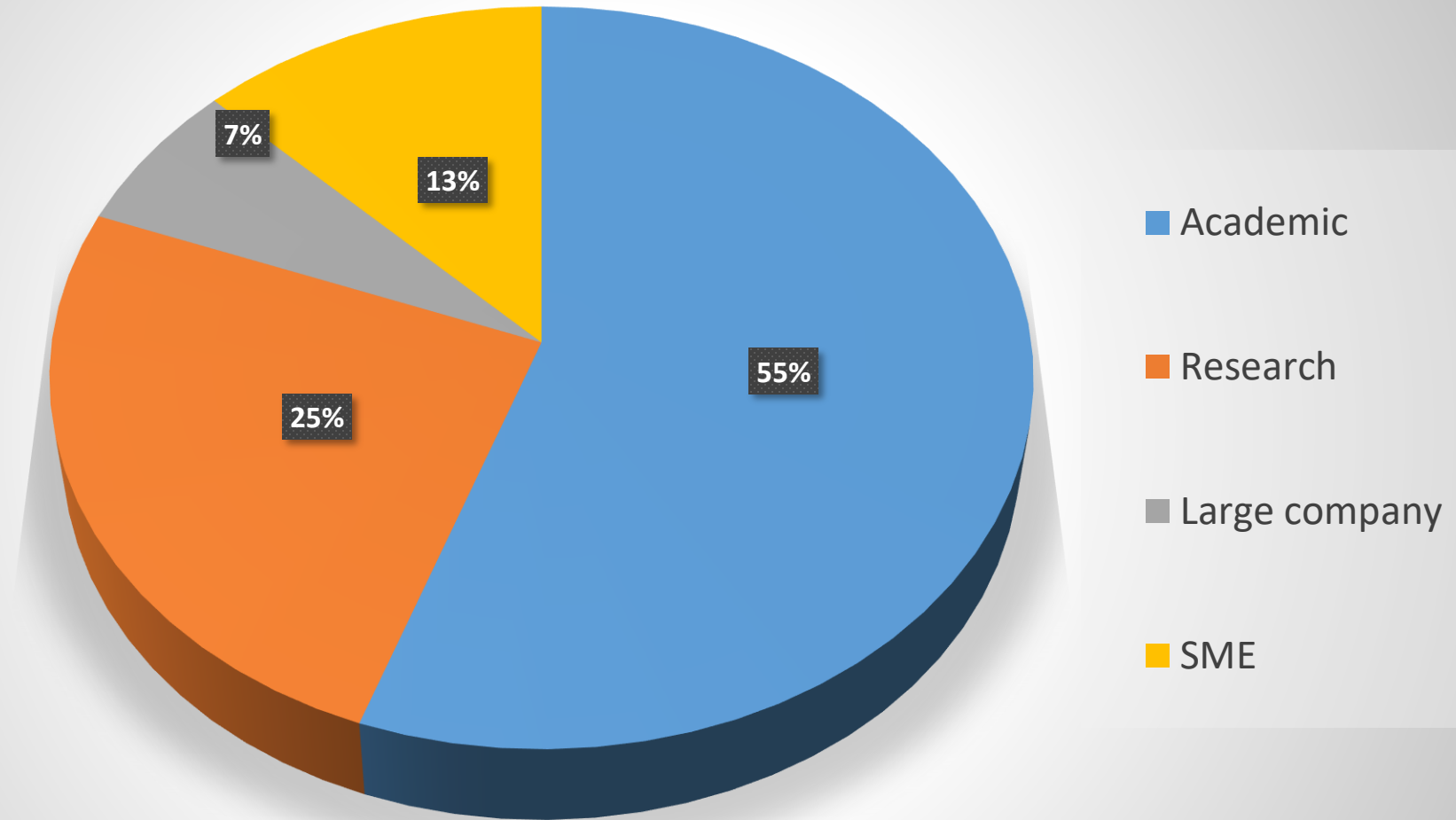
* Based on data collected for 161 POP Performance Audits



Application Sectors



Customer Types

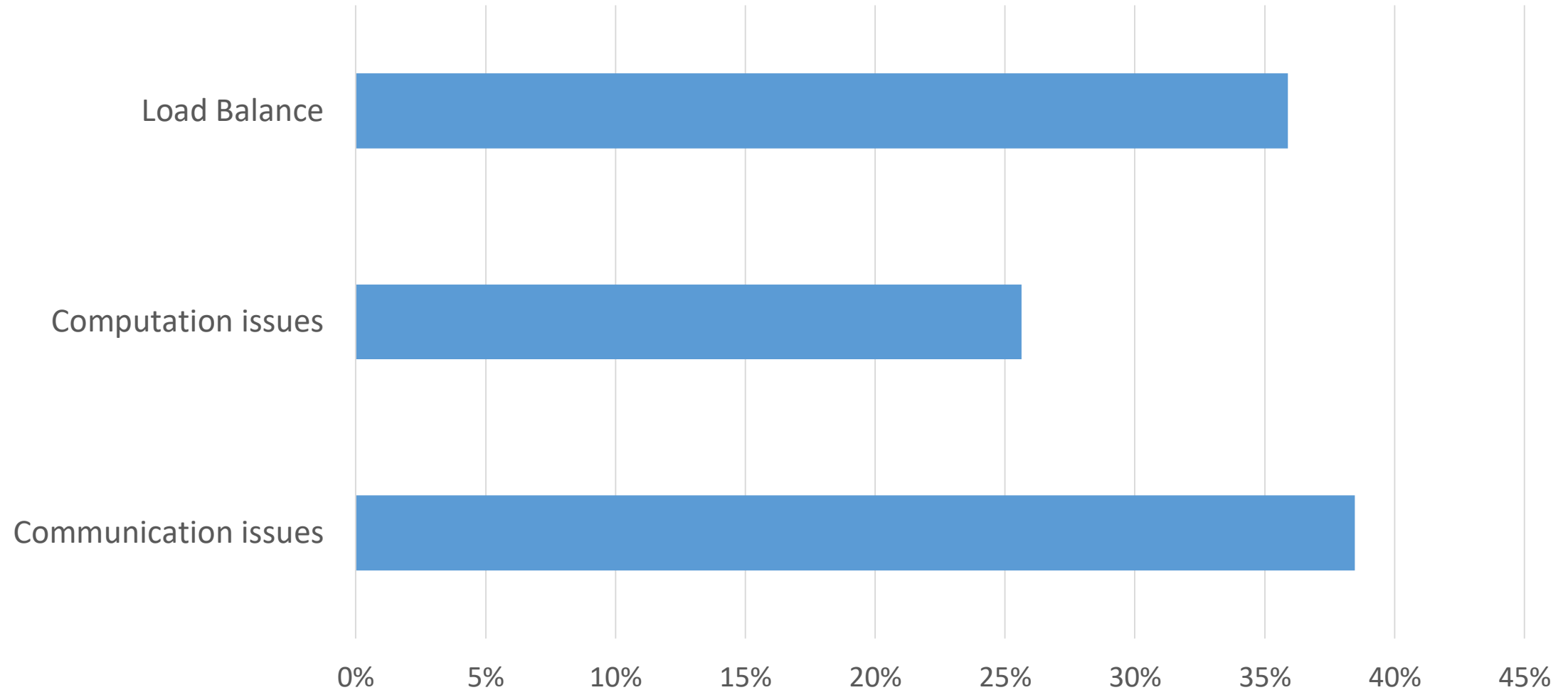




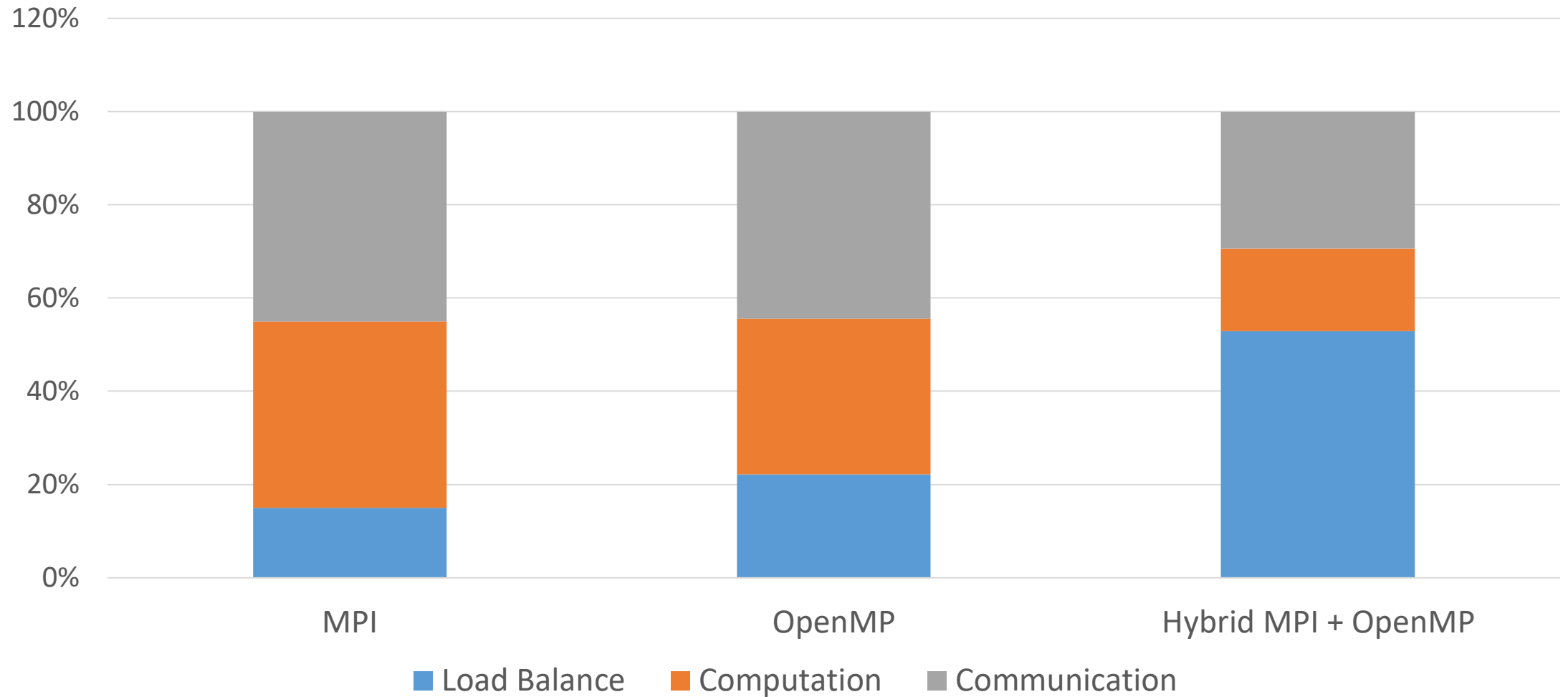
Analysis of Inefficiencies



Leading Cause of Inefficiency



Inefficiency by Parallelisation





Success Stories



Some PoC Success Stories



- See [⇒ https://pop-coe.eu/blog/tags/success-stories](https://pop-coe.eu/blog/tags/success-stories)



Performance Improvements for SCM's ADF Modeling Suite



3x Speed Improvement for zCFD Computational Fluid Dynamics Solver



25% Faster time-to-solution for Urban Microclimate Simulations



2x performance improvement for SCM ADF code



Proof of Concept for BPMF leads to around **40% runtime reduction**



POP audit helps developers **double their code performance**



10-fold scalability improvement from POP services



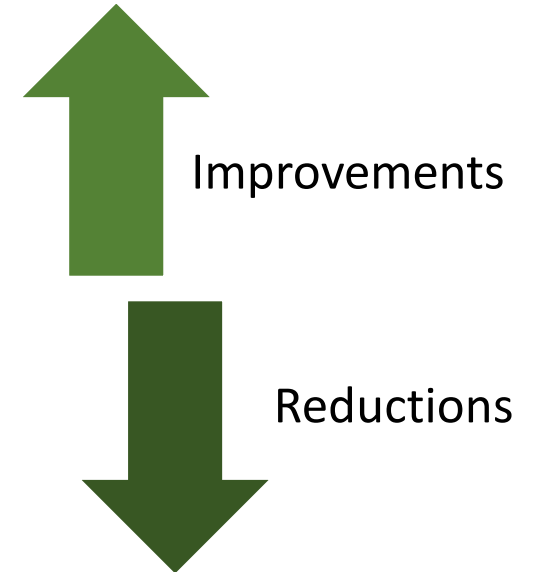
POP performance study improves performance **up to a factor 6**



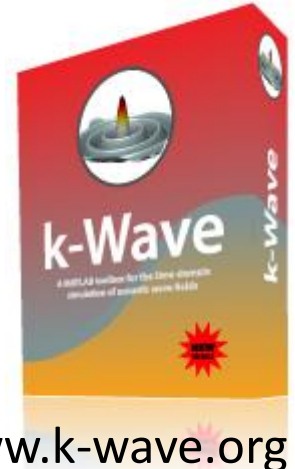
POP Proof-of-Concept study leads to **nearly 50% higher performance**



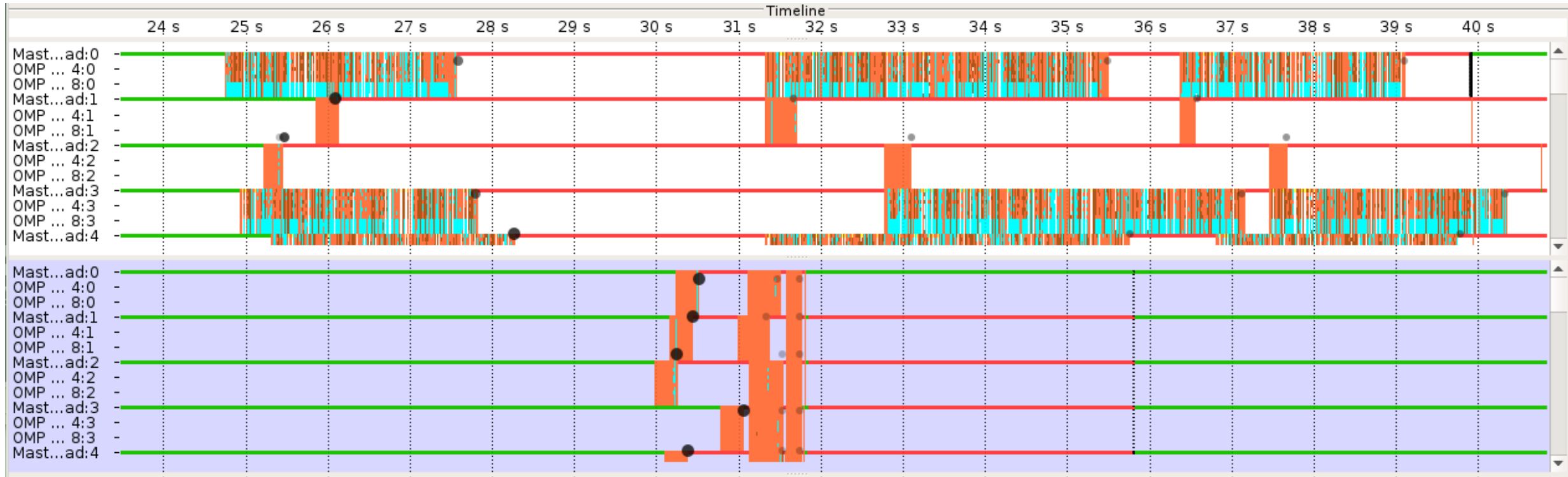
POP Proof-of-Concept study leads to **10X performance improvement** for customer



- Toolbox for time domain acoustic and ultrasound simulations in complex and tissue-realistic media
- C++ code parallelised with Hybrid MPI and OpenMP (+ CUDA)
- Executed on Salomon Intel Xeon compute nodes
- Key audit findings:
 - 3D domain decomposition suffered from major load imbalance : exterior MPI processes with fewer grid cells took much longer than interior
 - OpenMP-parallelised FFTs were much less efficient for grid sizes of exterior, requiring many more small and poorly-balanced parallel loops
- **Using a periodic domain with identical halo zones for each MPI rank reduced overall runtime by a factor of 2**

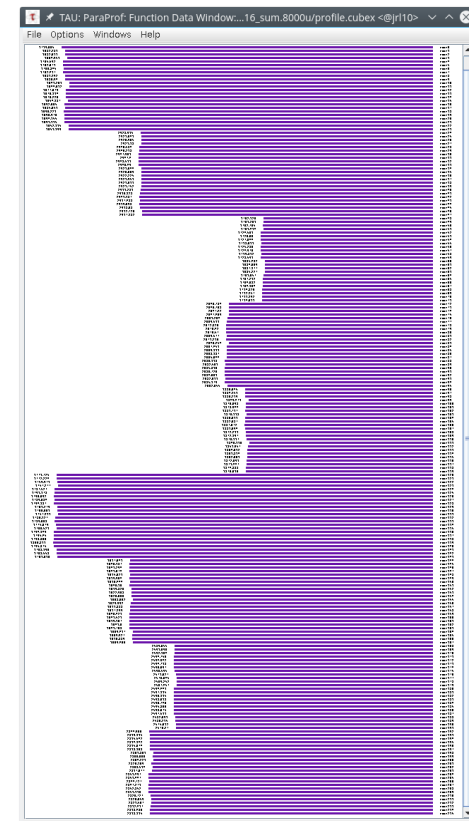


www.k-wave.org

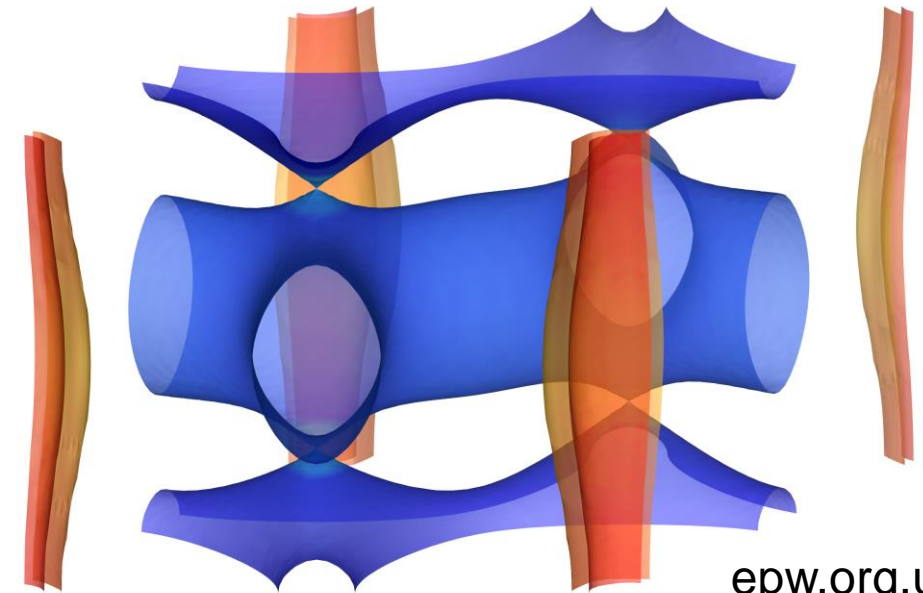


- Comparison time-line before (white) and after (purple) balancing, showing exterior MPI ranks (0,3) and interior MPI ranks (1,2)
 - User code in green, MPI synchronization in red, OpenMP synchronization in cyan

- Electron-Phonon Wannier (EPW) materials science DFT code;
- part of the Quantum ESPRESSO suite
- Fortran code parallelised with MPI
- Audit of unreleased development version of code
- Executed on ARCHER Cray XC30 (24 MPI ranks per node)
- Key audit findings:
 - Poor load balance from excessive computation identified
 - (addressed in separate POP Performance Plan)
 - Large variations in runtime, likely caused by IO
 - Final stage spends a great deal of time writing output to disk
- Report used for successful PRACE resource allocation



- Original code had all MPI ranks writing the result to disk at the end
- POP PoC modified this to have only one rank do output
- **On 480 MPI ranks, time taken to write results fell from over 7 hours to 56 seconds: 450-fold speed-up!**
- **Combined with previous improvements, enabled EPW simulations to scale to previously impractical 1920 MPI ranks**
- **86% global efficiency with 960 MPI ranks**



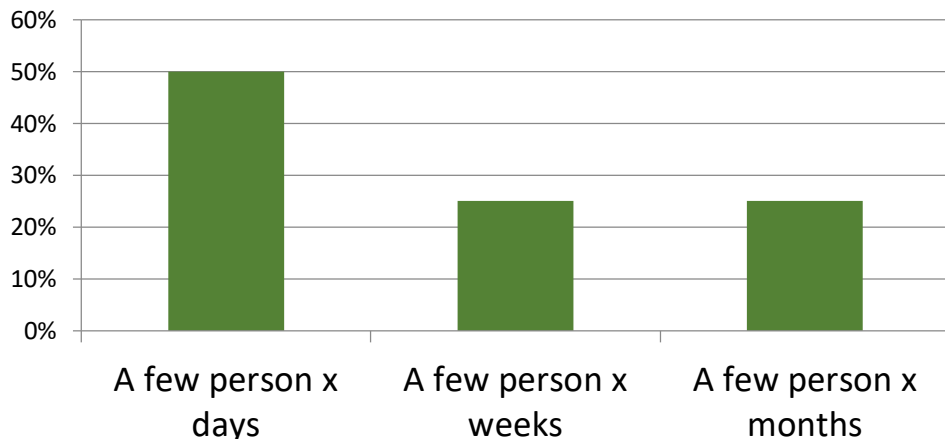
(Eight) Customers Success Feedback



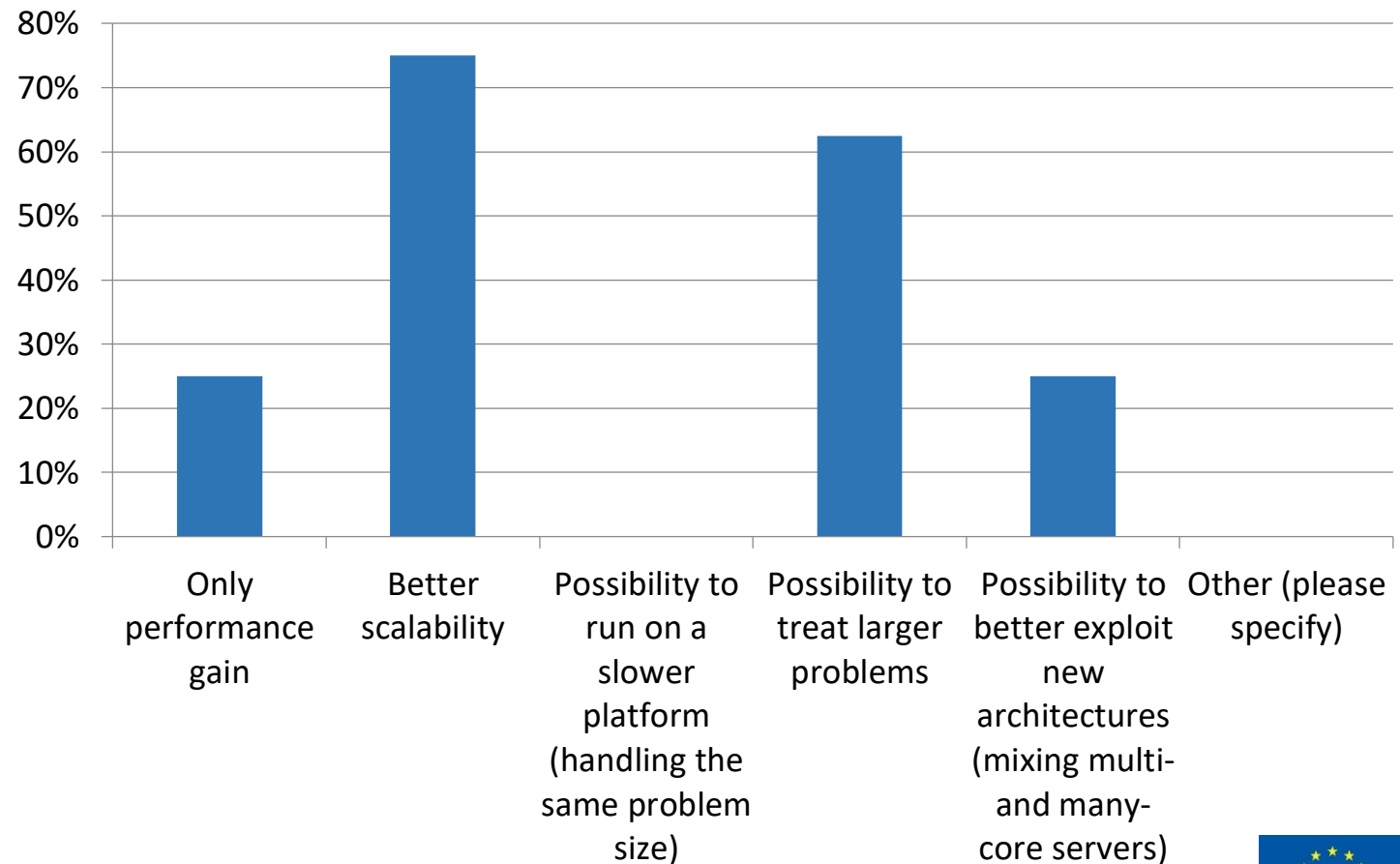
What is the observed performance gain after implementing recommendations?

25%
25%
20% overall, 50% for the given module
50-75% (case dependent)
12%
Up to 62 %, depending on the use case.
6 - 47 % depending on the test case.
15%

How much effort was necessary?



What are the main results?





Summary & Conclusion



Interactions with Leads

- 86% of users needed multiple interactions before signing up
 - Users with only 1 interaction referred by existing users
- Average number of interactions to sign up = 3.2
- Maximum number of interactions to sign up = 11

Conversions

- Over 1300 leads contacted throughout the project
- Conversion rate of 10.8% from leads to user
- Only 17 signed up without direct contact from POP

Customer Feedback



Performance Audits (73 customers)

- About 90% very satisfied or satisfied with service
- About half of the customers signed-up for a follow-up service

Performance Plans (11 customers)

- About 90% very satisfied or satisfied with service
- All customers thought suggestions were precise and clear and 70% plan to implement the suggested code modifications
- About 2/3 plan to do use the POP services again

Proof-of-Concepts (8 customers)

- All customers very satisfied or satisfied with this service
- About 80% plan to implement further code modifications or complete the work of the POP experts

* Based on data collected in 92 customer satisfaction questionnaires and 52 phone interviews with customers



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 Plan

- 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 \Rightarrow ROI of 620%

Summary & Conclusion (I)



- **POP CoE Phase 1 finished in March 2018** after 2½ years
 - **Successfully demonstrated expertise and impact**
 - 152 Audits + Perf Plans / 22 Proof-of-Concept / 21 requests cancelled
 - 158 closed / 16 in progress
 - **Intensive dissemination** via website, blog articles, tweets, newsletter, ...
 - ⇒ Expected more interest from industry / SME / ISVs
- **POP CoE Phase 2 restarted in December 2018** for 3 more years
 - New Service Structure (Performance Assessment combines Audit and Plan)
 - New Project Partners (IT4I, UVSQ)
 - New Co-design Data Repository
 - Extension of Efficiency Model: Vectorization, I/O, GPUs, ...



Summary & Conclusion (II)



- Issues identified
 - **FREE (Money) \neq FREE (Efforts, Time)**
 - To much(?) customer effort (providing code, input, measurements?, feedback)
 - Desire to serve more industrial customers / SMEs, **BUT**
 - Resistance for allowing us to publish their results / success stories
 - Almost every time require NDA agreements
- Sustainability
 - Real costs audit (EUR 16K-18K) >> Price customer would pay (5K-7K)





Dissemination and Contact



- POP User Portal
- Access to all public information and services

The screenshot shows the POP website homepage. At the top, the POP logo is followed by the text "Performance Optimisation and Productivity" and "A Centre of Excellence in HPC". A "Log in" button is in the top right. On the left, a sidebar menu contains links for News, Blog, Newsletter, Events, Partners, Tools, Services, Request Service Form, Target Customers, Success Stories, Customer Code List, Further Information, Learning Material, Contact, and Privacy Policy. Below the menu is a "Subscribe to our Newsletter" section with an email input field and a "Subscribe" button. The main content area features a "Mission" section, a "Blog Highlights" section with three entries, and a "Latest News" section with social media links and a tweet feed. A red stamp in the top right corner reads "Latest News: POP RESTARTED Dec 1, 2018!".

POP Performance Optimisation and Productivity
A Centre of Excellence in HPC

Log in

News

- Blog
- Newsletter
- Events

Partners

- Tools

Services

- Request Service Form
- Target Customers
- Success Stories
- Customer Code List

Further Information

- Learning Material

Contact

- Privacy Policy

Subscribe to our Newsletter

Write your e-mail ...

☐ I accept the data policy *

Subscribe

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!

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

POP ? WORK ! SUCCESS

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 [LinkedIn group](#)

Tweets by @POP_HPC

POP_HPC @POP_HPC

Come be a part of this great project! UK based job.

Jan 31, 2019

POP_HPC @POP_HPC

Wishes a Performance and Optimized 2019!

Blog – <https://pop-coe.eu/blog>



- Typically 2 new articles per month
- Easy filtering via Tags, e.g.
 - Success Stories
 - Events
 - Webinars
 - ...
- RSS feed
 - <https://pop-coe.eu/blog/rss>

The screenshot shows the POP (Performance Optimisation and Productivity) Blog page. The header features the POP logo and the text "Performance Optimisation and Productivity" and "A Centre of Excellence in Computing Applications". A "Log in" button is in the top right. Below the header, there's a navigation menu with "News" selected. The main content area is titled "Blog" and lists several articles with dates, icons, and titles. The right sidebar contains "Tags" (Award, Events, Metrics, Partner profile, Performance tools, POP Project, Services, Success Stories, Webinar) and "Last posts" (07 FEB 5th POP Webinar, 25 JAN Not Only Fortran and MPI, 24 JAN POP @ HIPEAC18, 13 DEC Performance Improvements for SCM's ADF Modeling Suite, 04 DEC 4th POP Webinar). A "Subscribe to our Newsletter" form is at the bottom left of the main content area.

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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 DI
[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 Kenned
[READ MORE](#)

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
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EU H2020 funded Centre of Excellence Performance Optimization and Productivity (POP) to boost performance and productivity in HPC applications.

pop-coe.eu

Joined October 2016

Born on October 1, 2000

Tweets Tweets & replies Media

Pinned Tweet

POP_HPC @POP_HPC · Oct 19

Our aim is to help you optimise your parallel code. Do bigger, better, faster science with POP. pop-coe.eu

POP_HPC @POP_HPC · 2h

Who to follow · Refresh · View all

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Horizon 2020 @Horizon20...
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Follow

martorellBSC @martorellB...
Followed by EXDCI and oth...
Follow



LinkedIn Group



LinkedIn interface showing the Performance Optimization and Productivity (POP) group page. The page includes a search bar, navigation icons (Home, My Network, Jobs, Messaging, Notifications, Me), and a premium offer. The group is owned by Bernd Mohr and has 80 members. A post by Jonathan Boyle, HPC Application Analyst at NAG, is featured, titled "POP webinar - Large-scale Application Execution Performance Assessment". The post includes a video thumbnail and a line graph showing speed-up versus runtime reduction for various code configurations.

Performance Optimization and Productivity (POP)
Standard group

Jonathan Boyle • 1st
HPC Application Analyst at NAG
6mo

POP webinar - Large-scale Application Execution Performance Assessment

Thursday 7 June 2018 14:00hrs BST | 15:00hrs CEST ...see more

7th POP Webinar - Large-Scale Application Execution Performance Assessment
pop-coe.eu

1 Like

Like Comment

Wadud Miah • 1st
Computational Scientist at Numerical Algorithms Group
9mo

POP highlights improvements in Shearwater Reveal seismic processing code of up to 44% runtime reduction

Speed-up

12
10
8
6
4
2

Linear (CPU scaling)
80% of linear (CPU scaling)
PoC code - dynamic
PoC code - I/O and alloc/dealloc removed
original code - static

POP highlights improvements in Shearwater Reveal seismic processing code of up to 44% runtime reduction

- Important announcements
- Serves also as user forum



Quarterly Email Newsletter




- Subscribe on POP website
- Newsletter archive: <https://pop-coe.eu/news/newsletter>

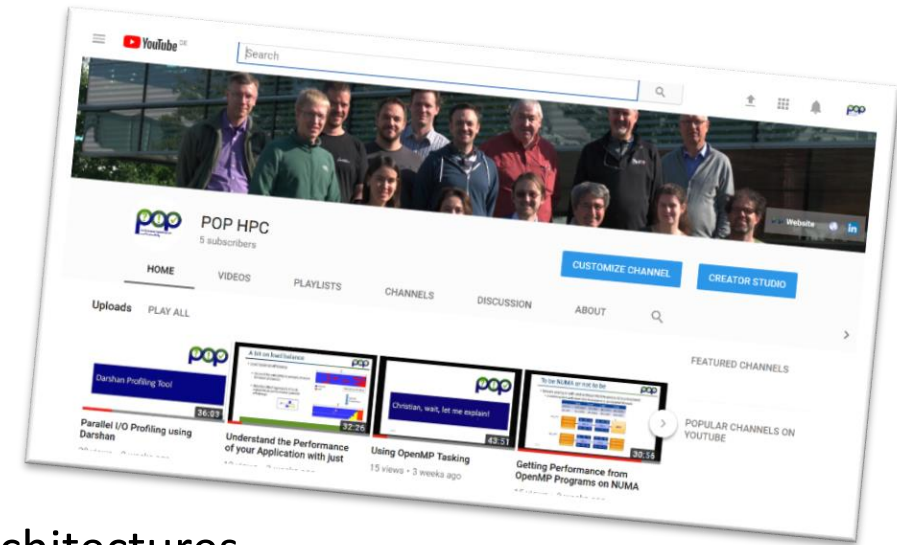
The screenshot shows the first page of the POP Newsletter. It features the POP logo and the title 'Performance Optimisation and Productivity - A Centre of Excellence in Computing Applications'. The main heading is 'POP Newsletter 1 -- Issue June 2016'. Below this, there is a table of contents with links to various sections: 'Welcome', 'The POP CoE Vision', 'The POP CoE Services', 'POP Partner Profiles', 'POP's Performance Analysis Tools', and 'Meet POP CoE partners at some upcoming events'. The 'Welcome' section includes a list of topics covered in the newsletter, such as 'An overview of the POP CoE vision', 'A description of our services', 'Profiles of the members of the POP consortium', 'Highlights from our recent performance analysis', and 'An analysis of service requests to date'.

The screenshot shows the 'POP Partner Profiles' section of the newsletter. It features a heading 'POP Partner Profiles' and a sub-heading 'The Numerical Algorithms Group (NAG)'. The text describes the NAG's history and its role in the POP CoE. It mentions that the NAG was founded in 1970 as a collaboration between the universities of Birmingham, Leeds, Manchester, Nottingham and Oxford, and that it is now known as the Numerical Algorithms Group. The text also highlights the NAG's expertise in numerical software, consulting, and high-performance computing. A photograph of the NAG team is included. Below this, there is a section for 'The HPC Group at RWTH Aachen', which describes the group's focus on high-performance computing and its role in the POP CoE. A photograph of the HPC Group team is also included.

The screenshot shows the 'new thing just - 10x improvement for Optimix Code' section of the newsletter. It features a heading 'new thing just - 10x improvement for Optimix Code' and a sub-heading 'Breakdown of our users' codes'. The text describes the results of a performance analysis conducted by the POP CoE. It mentions that the analysis was conducted on 100 code samples and that it resulted in a 10x improvement in performance for the Optimix Code. A table of results is included, showing the breakdown of the users' codes by language and by type of application. The table shows that the majority of the codes are written in C++ and that they are primarily used for scientific and engineering applications. Below the table, there is a section for 'Meet POP CoE partners at some upcoming events', which lists several events and provides information on how to attend them.



- See [⇒ https://pop-coe.eu/blog/tags/webinar](https://pop-coe.eu/blog/tags/webinar)
- Or see our  channel youtube.com/POPHPC
- Already available:
 - How to Improve the Performance of Parallel Codes
 - Using OpenMP Tasking
 - Parallel I/O Profiling Using Darshan
 - Getting Performance from OpenMP Programs on NUMA Architectures
 - Understand the Performance of your Application with just Three Numbers
 - The impact of sequential performance on parallel codes
 - Large scale Application Execution Performance Assessment
 - POP Case Study: 3x Speed Improvement for Zenotech's zCFD Solver
 - Exascale Matrix Factorization: Using HPC and ML for Drug Discovery
 - Software for Linear Algebra Targeting Exascales (SLATE) Project
 - Implementing I/O Best Practices to Improve System Performance with Ellexus





Performance Optimisation and Productivity

A Centre of Excellence in HPC

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