



# Parallel Performance Optimization and Productivity

EU H2020 Centre of Excellence (CoE)

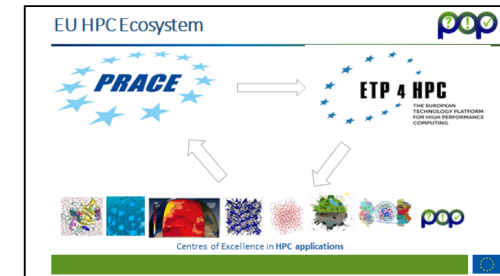


Grant Agreement No 824080

1 December 2018 – 30 November 2021



- 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 !**



# Partners



## • 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

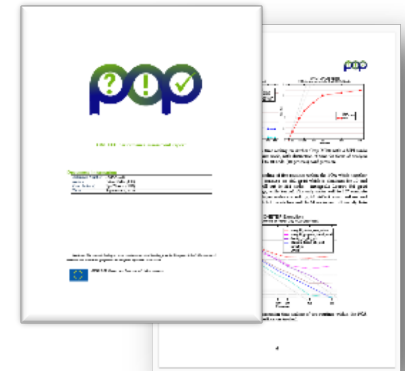


# FREE Services provided by the CoE



- **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!

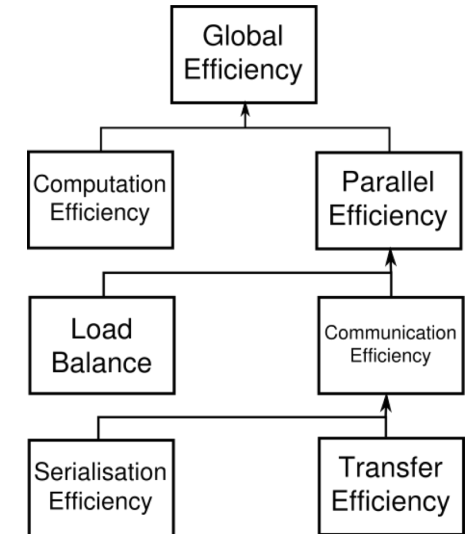




# Efficiencies



- 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



CT = Computational time  
TT = Total time

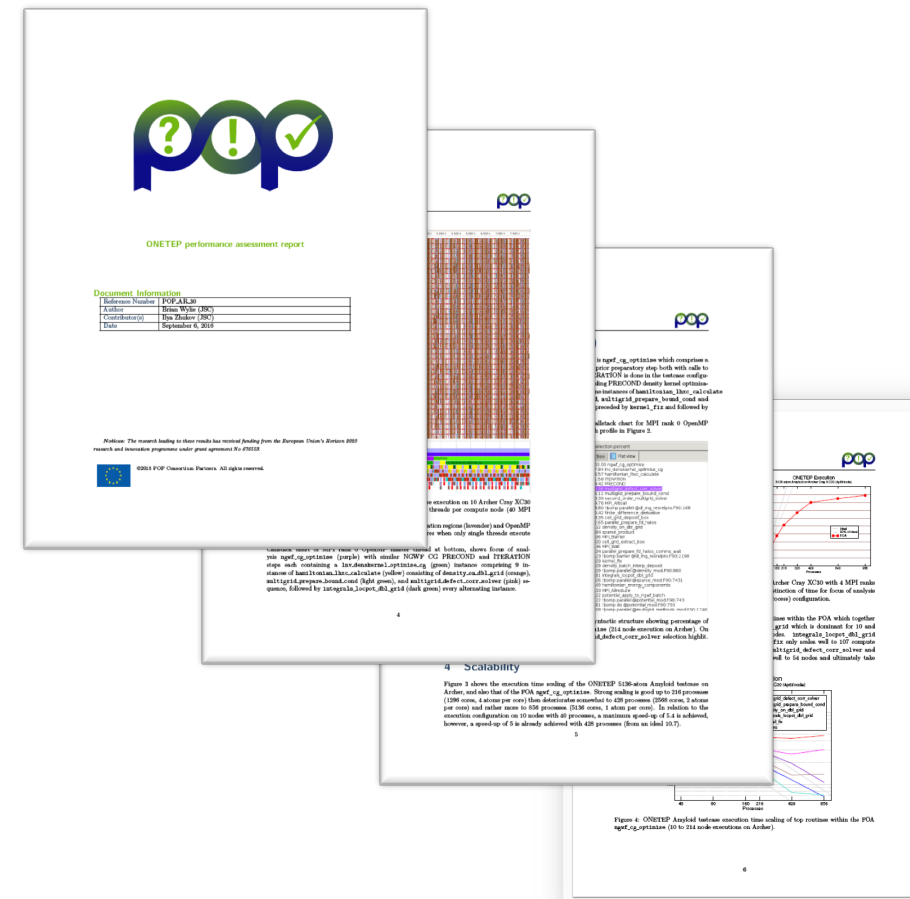
- Details see <https://sharepoint.ecampus.rwth-aachen.de/units/rz/HPC/public/Shared%20Documents/Metrics.pdf>



# 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



- **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

# Target customers



- **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



# 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](mailto:pop@bsc.es)
- Selection/assignment process
- Install tools @ your production machine (local, PRACE, ...)
- Interactively: Gather data → Analysis → Report





# 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

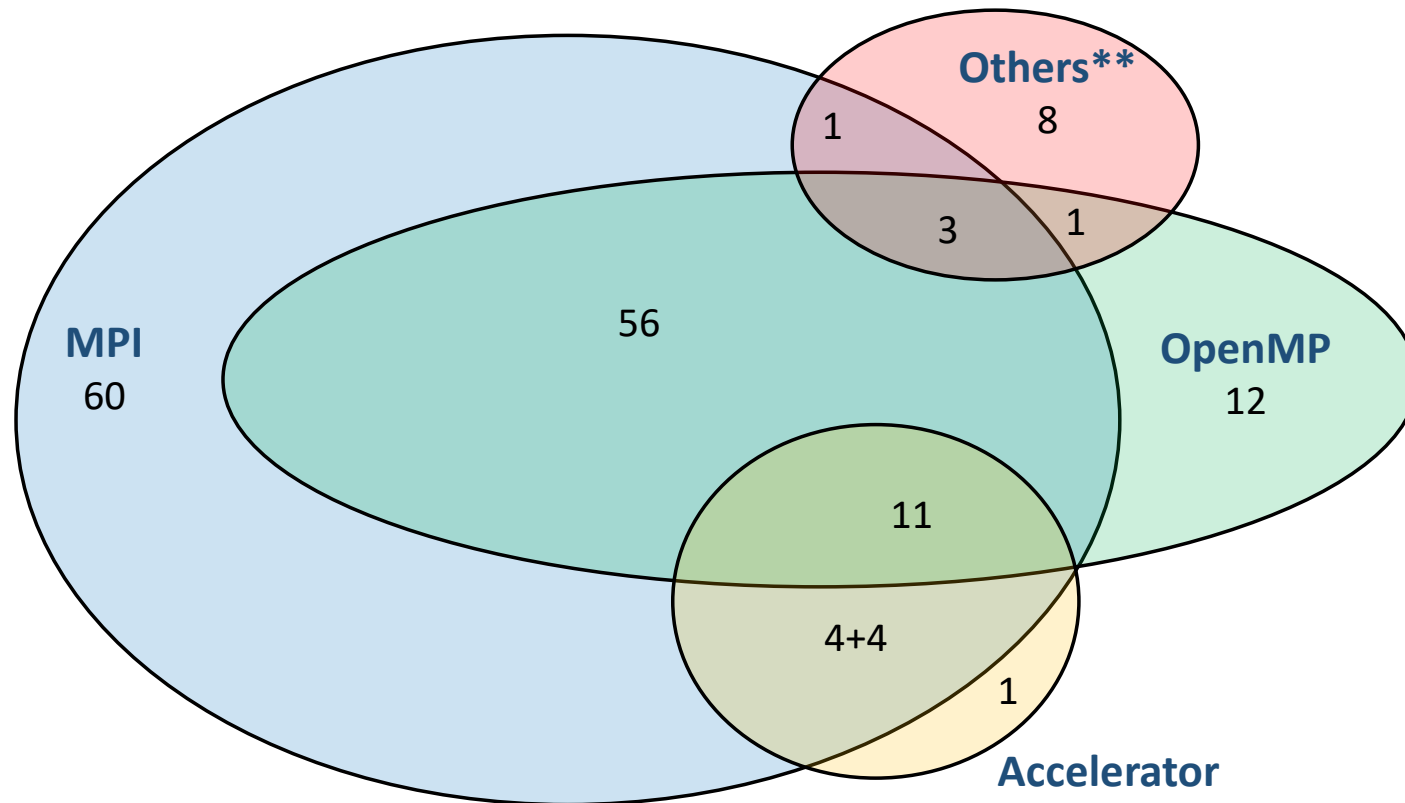


Area	Codes
Computational Fluid Dynamics	DROPS (RWTH Aachen), Nek5000 (PDC KTH), SOWFA (CENER), ParFlow (FZ-Juelich), FDS (COAC) & others
Electronic Structure Calculations	ADF, BAND, DFTB (SCM), Quantum Espresso (Cineca), FHI-AIMS (University of Barcelona), SIESTA (BSC), ONETEP (University of Warwick)
Earth Sciences	NEMO (BULL), UKCA (University of Cambridge), SHERAT-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), GraGLoS2D (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

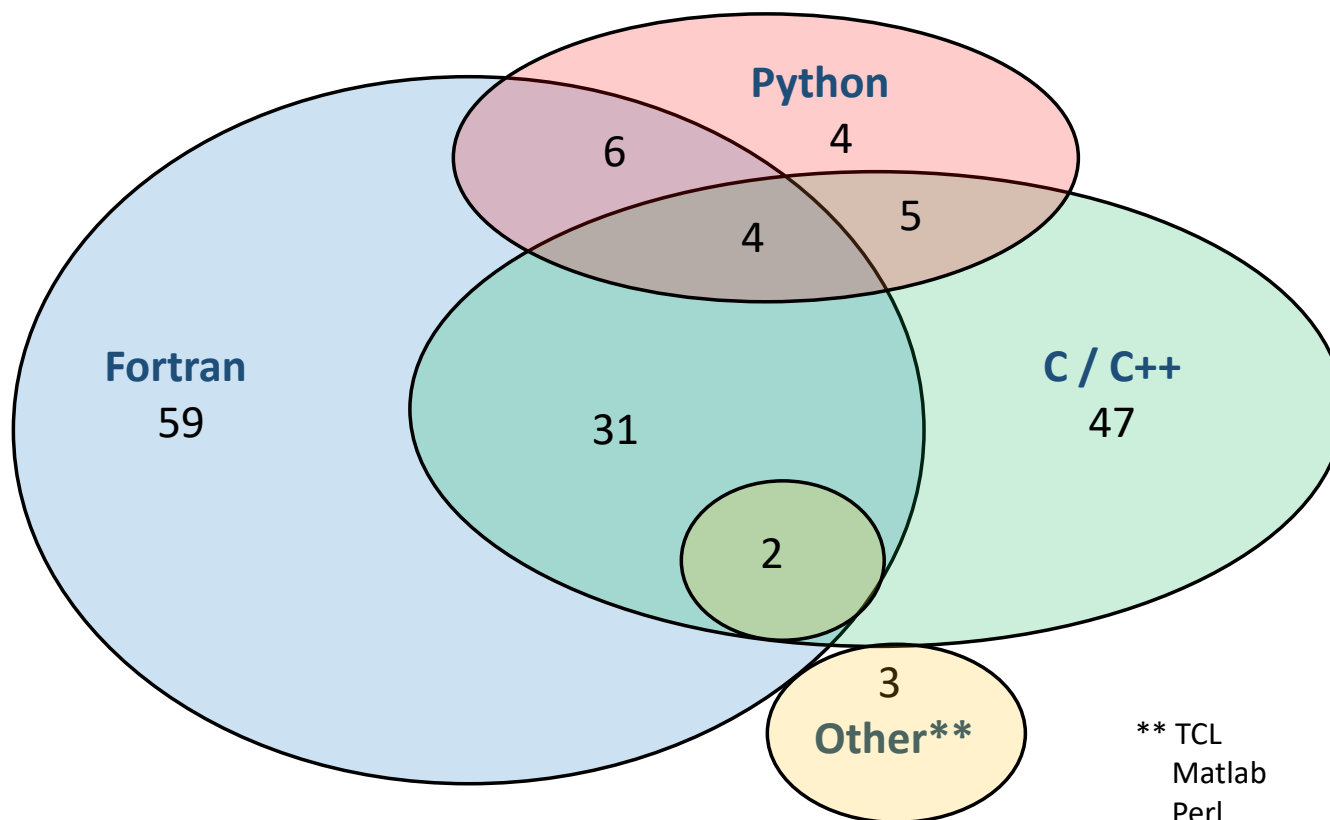


\*\* MAGMA  
Celery  
TBB  
GASPI  
C++ threads  
MATLAB PT  
StarPU  
GlobalArrays  
Charm++  
Fortran Coarray

\* Based on data collected for 161 POP Performance Audits



# Programming Languages Used

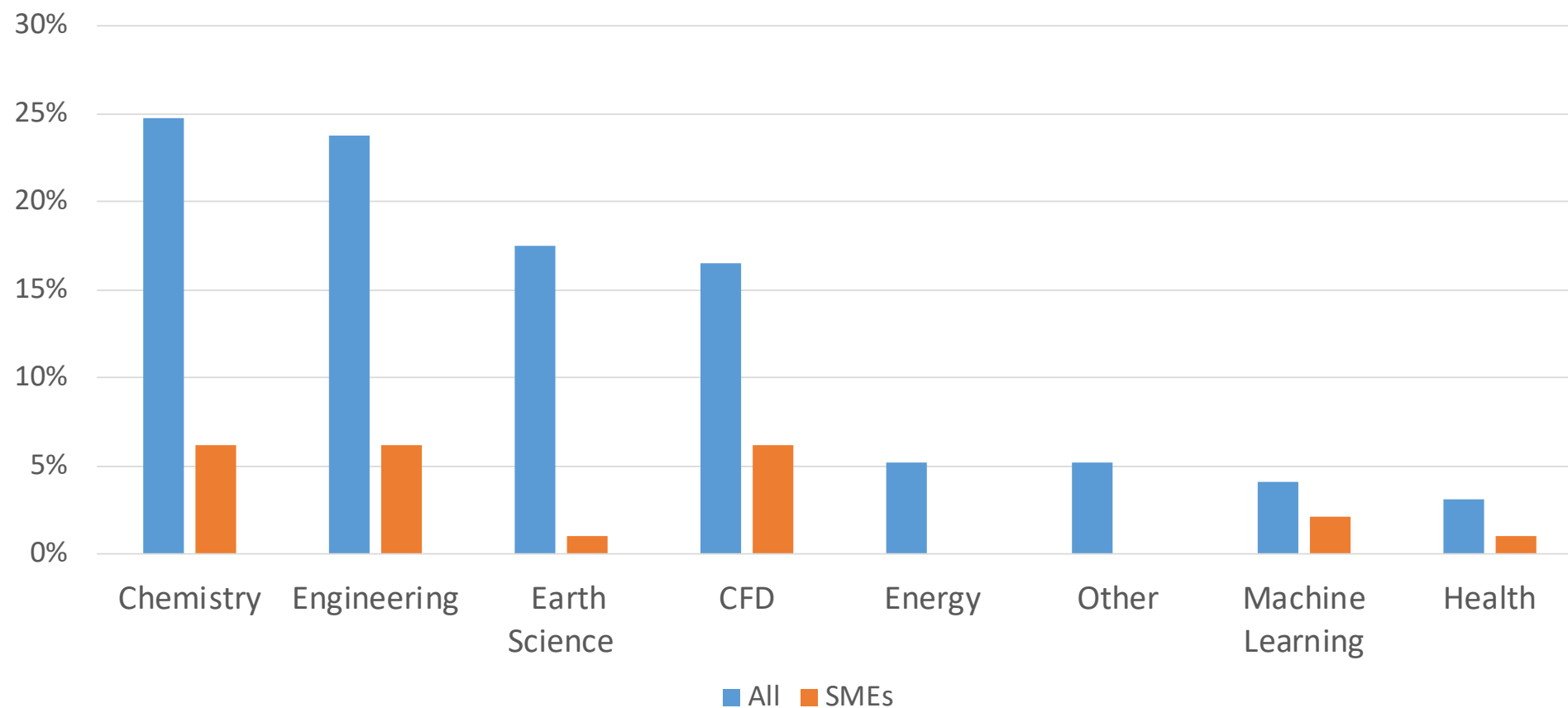


\*\* TCL  
Matlab  
Perl  
Octave  
Java

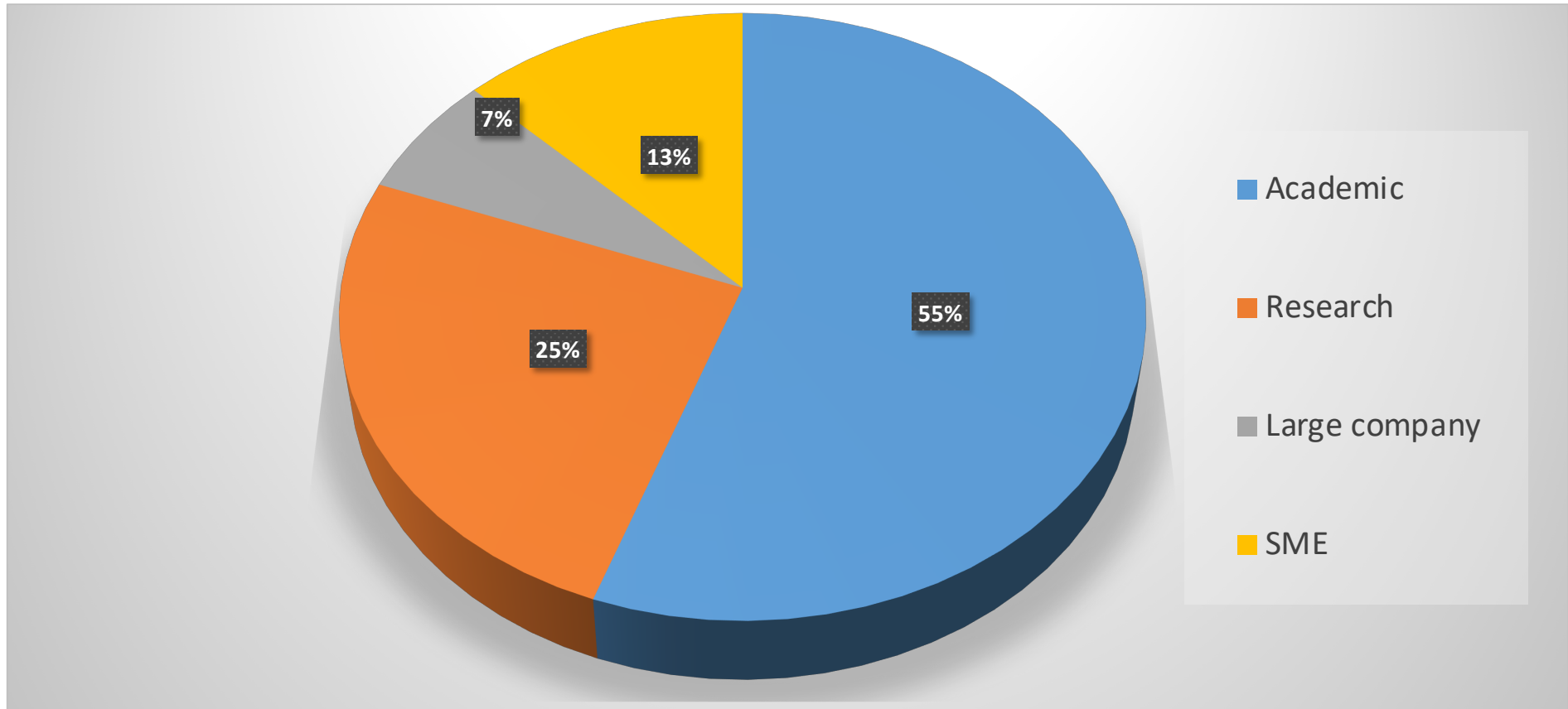
\* Based on data collected for 161 POP Performance Audits



# Application Sectors



# Customer Types

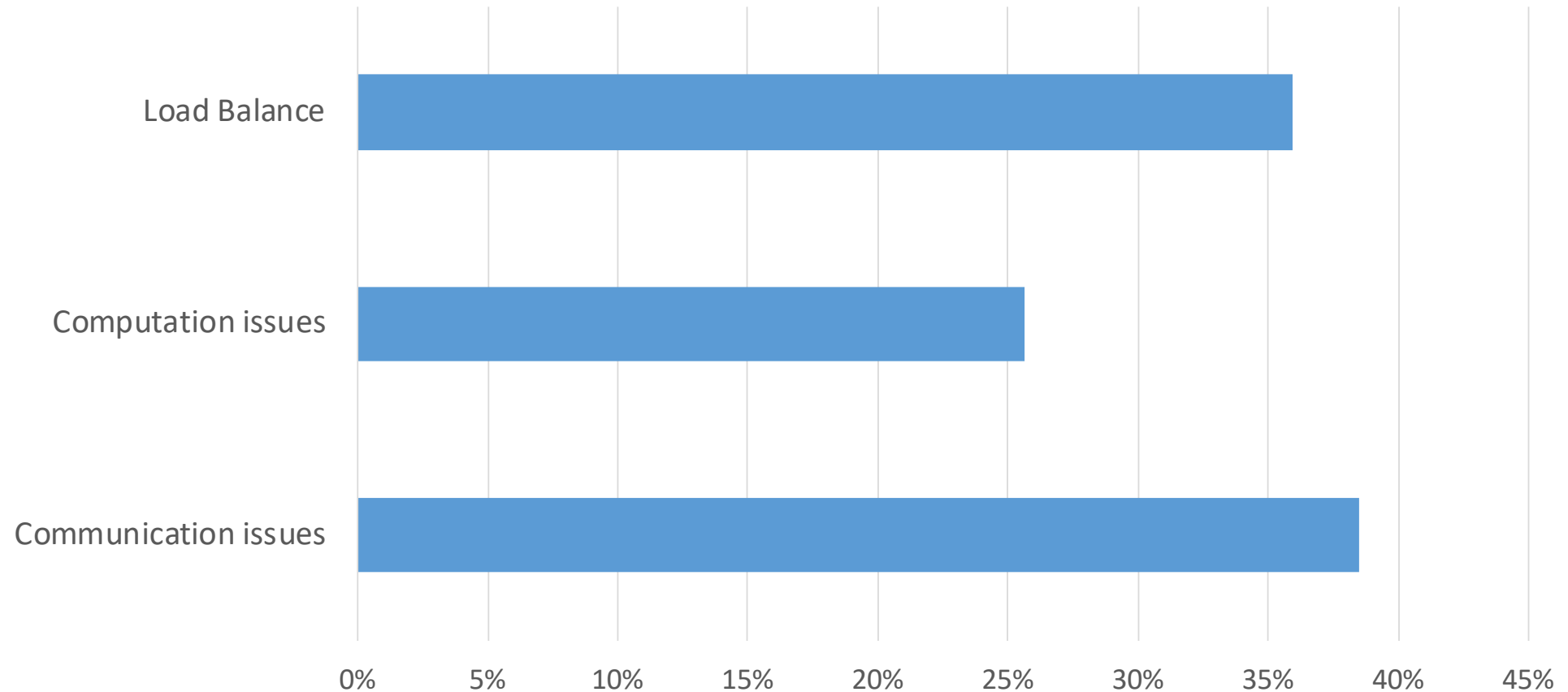




# Analysis of Inefficiencies



# Leading Cause of Inefficiency





# 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



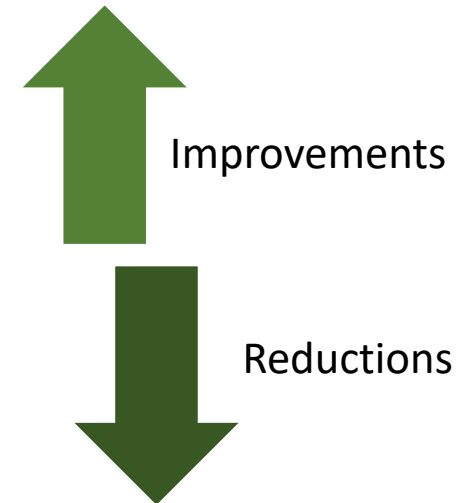
POP performance study improves performance **up to a factor 6**



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



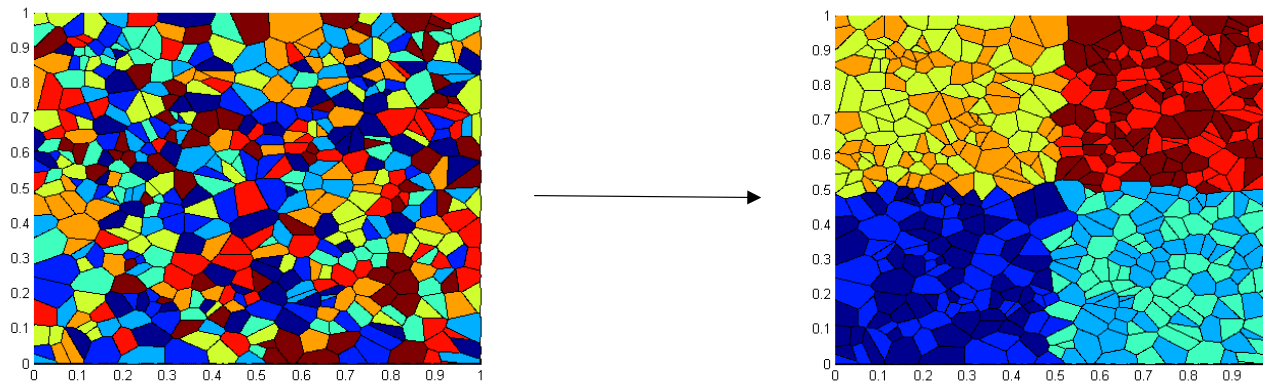
POP Proof-of-Concept study leads to **10X performance improvement** for customer





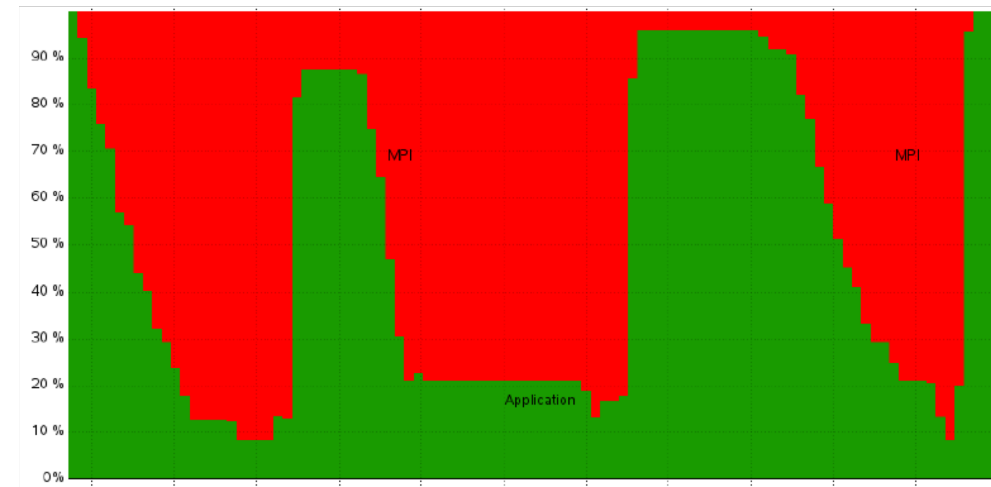
- Simulates grain growth phenomena in polycrystalline materials
- C++ parallelized with OpenMP
- Designed for very large SMP machines (e.g. 16 sockets and 2 TB memory)
- **Key audit results:**
  - **Good load balance**
  - **Costly use of division and square root inside loops**
  - **Not fully utilising vectorisation in key loops**
  - **NUMA data sharing issues lead to long times for memory access**

- Improvements:
  - Restructured code to enable vectorisation
  - Used memory allocation library optimised for NUMA machines
  - Reordered work distribution to optimise for data locality



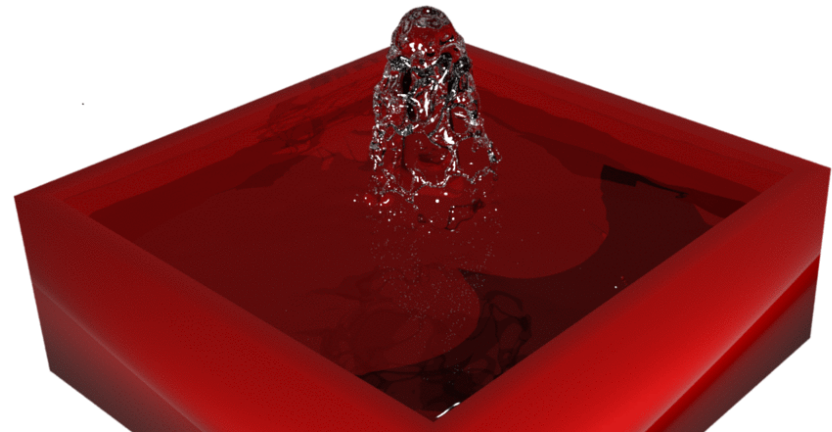
- Speed up in region of interest is more than 10x
- Overall application speed up is 2.5x

- Finite element code
- C and Fortran code with hybrid MPI+OpenMP parallelisation
- **Key audit results:**
  - **High number of function calls**
  - **Costly divisions inside inner loops**
  - **Poor load balance**
- Performance plan:
  - Improve function inlining
  - Improve vectorisation
  - Reduce duplicate computation



- Inlined key functions → **6% reduction in execution time**
- Improved mathematical operations in loops → **28% reduction in execution time**
- Vectorisation: found bug in gnu compiler, confirmed Intel compiler worked as expected
- **6 weeks software engineering effort**
- **Customer has confirmed “substantial” performance increase on production runs**

- Simulates fluids for computer graphics applications
- C++ parallelised with OpenMP
- Key audit results:
  - Several issues relating to the sequential computational performance
  - Located critical parts of the application with specific recommended improvements

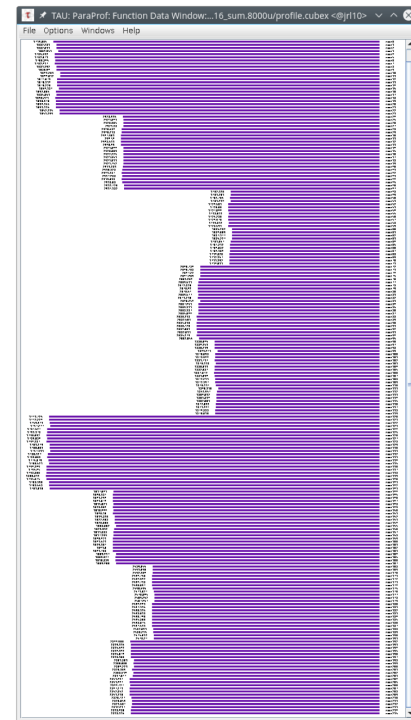
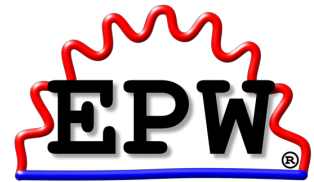


- Implemented by the code developers:
  - Review of overall code design from issues identified in POP audit
  - Inlining short functions
  - Reordering the particle processing order to reduce cache misses
  - Removal of unnecessary operations and costly inner loop definitions
- **Confirmed performance improvement up to 5x – 6x depending on scenario and pressure model used**
- Used insights provided by the POP experts and the good information exchange during the work

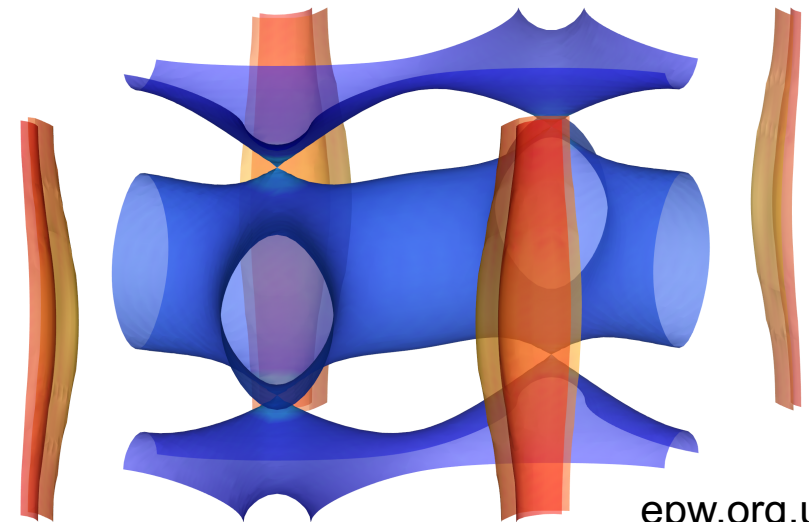
# EPW – University of Oxford



- 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**





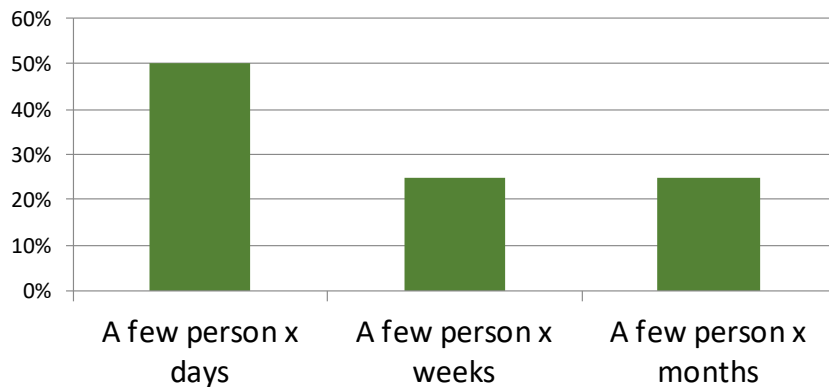
# (Eight) Customers Success Feedback



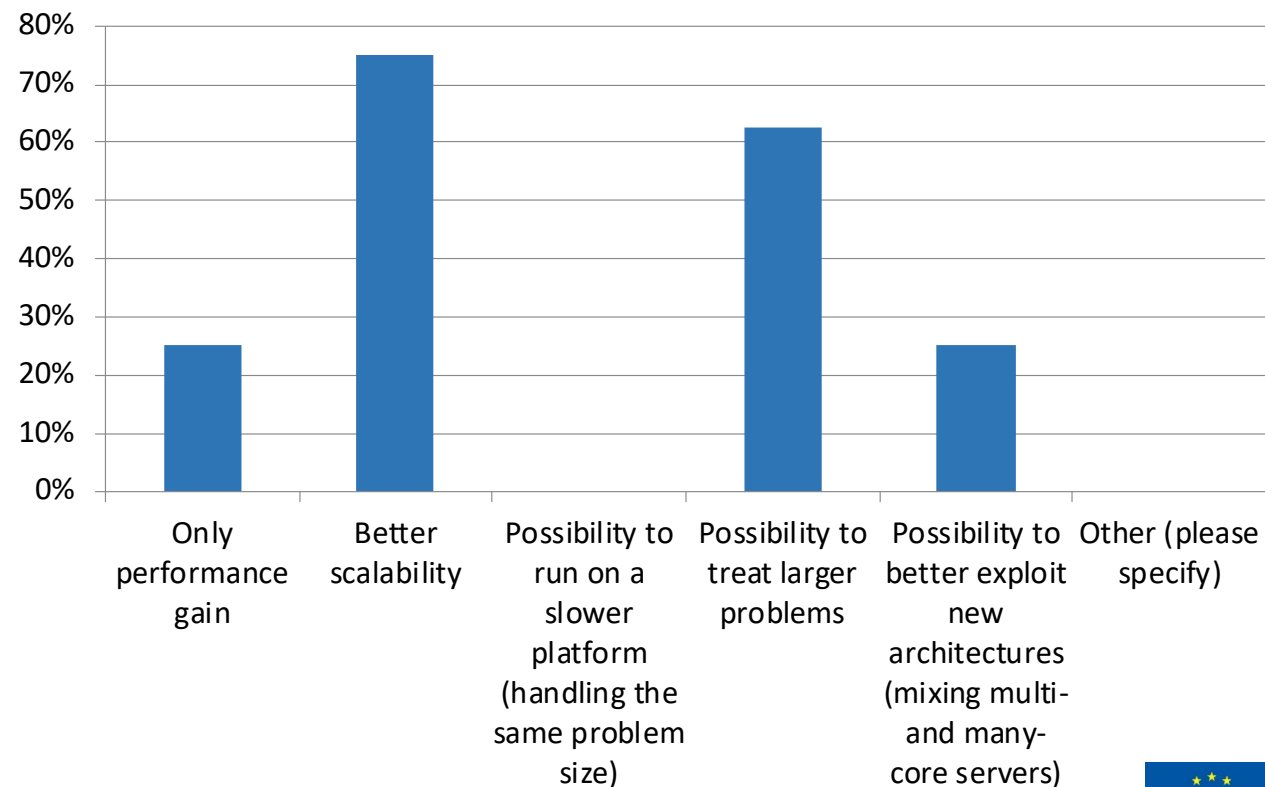
**What is the observed performance gain after implementing recommendations?**

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



# 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



# ROI 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 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%





# Dissemination and Contact



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



- 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 corner. On the left, a vertical menu lists: 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, a checkbox for "I accept the data policy", and a "Subscribe" button. The main content area features a "Mission" section, a "Blog Highlights" section with three entries, and a "Latest News" section. A red stamp in the top right corner of the page reads "Latest News: POP RESTARTED Dec 1, 2018!". The "Blog Highlights" section includes entries for December 1st (POP Project Restarted), January 25th (Not Only Fortran and MPI), and December 6th (Standard metrics for parallel performance analysis). The "Latest News" section includes social media links for Twitter, YouTube, and LinkedIn, and a "Tweets by @POP\_HPC" section showing a tweet about the project restart.

**POP** Performance Optimisation and Productivity  
A Centre of Excellence in HPC

Log in

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☐ 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 Optimised 2019!

12-Dec-2018



# Blog – <https://pop-coe.eu/blog>



- Typically 2 new articles per month
- Easy filtering via Tags, e.g.
  - Success Stories
  - Events
  - Webinars
  - ...

The screenshot shows the POP (Performance Optimisation and Productivity) blog homepage. 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. A navigation menu on the left includes "News", "Blog", "Newsletter", "Events", "Partners", "Tools", "Services", "Request Service Form", "Target Customers", "Success Stories", "Customer Code List", "Further Information", "Learning Material", and "Contact". Below the menu is a "Subscribe to our Newsletter" section with an email input field and a "Subscribe" button. The main content area is titled "Blog" and lists several articles with their dates, icons, titles, and "READ MORE" links. The articles include: "5th POP Webinar - Parallel I/O Profiling Using Darshan" (07 FEB), "Not Only Fortran and MPI: POP's View of HPC Software in Europe" (25 JAN), "POP @ HIPEAC18" (24 JAN), "Performance Improvements for SCM's ADF Modeling Suite" (13 DEC), "4th POP Webinar - Using OpenMP Tasking" (04 DEC), "3x Speed Improvement for Zenotech's zCFD Computational Fluid Dynamics Solver" (22 NOV), and "POP Coordinator Jesus Labarta wins ACM and IEEE Computer Society Award" (15 NOV). A "Tags" section on the right lists "Award", "Events", "Metrics", "Partner profile", "Performance tools", "POP Project", "Services", "Success Stories", and "Webinar". A "Last posts" section lists the same articles in reverse chronological order.

12-Dec-2018

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# Follow us on Twitter @POP\_HPC





# LinkedIn Group



The screenshot shows the LinkedIn group page for 'Performance Optimization and Productivity (POP)'. The group is owned by Bernd Mohr and has 80 members. The page features a sidebar with navigation options like 'Home', 'My Network', 'Jobs', 'Messaging', 'Notifications', and 'Me'. The main content area displays a post by Jonathan Boyle about a 'POP webinar - Large-scale Application Execution Performance Assessment' held on Thursday 7 June 2018. The post includes a video thumbnail and a line graph showing speed-up results. The graph compares five scenarios: Linear (CPU scaling), 80% of linear (CPU scaling), PoC code - dynamic, PoC code - I/O and alloc/dealloc removed, and original code - static. The PoC code variants show significant improvements in speed-up, reaching up to 12x for the dynamic version. Below the graph, a caption states: 'POP highlights improvements in Shearwater Reveal seismic processing code of up to 44% runtime reduction'. The right sidebar provides information about the group, including its description as the EU H2020 Performance Optimisation and Productivity (POP) Centre of Excellence (CoE) and lists the group owner (Bernd Mohr) and manager (Jonathan Boyle).

**Performance Optimization and Productivity (POP)**

Standard group

80 members

Invite members

About this group

The EU H2020 Performance Optimisation and Productivity (POP) Centre of Excellence (CoE) in Computing Applications provides performance optimisation and productivity services for academic AND industrial HPC code(s) in all domains! The services are free of charge to organisations in the EU!

Show more

Group owner

Bernd Mohr · You  
Deputy Division Head at Jülich Supercomputing Centre

Group manager

Jonathan Boyle · 1st  
HPC Application Analyst at NAG

POP webinar - Large-scale Application Execution Performance Assessment

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

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

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

Speed-up

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



- 12-Dec-2018

[illegible]

# Webinars / YouTube



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

- Or see our  [YouTube Channel](#)

- Already 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





# Performance Optimisation and Productivity

A Centre of Excellence in HPC

Contact:

<https://www.pop-coe.eu>

<mailto:pop@bsc.es>

 @POP\_HPC

