



D2.3 First Business Development and Sustainability Review Version 1.0

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Executive Summary

This document describes the business development activity of the POP Project. We detail the marketing activities and collaborations we have undertaken and how they relate to our goals of working with SMEs and other Horizon 2020 Centres of Excellence (CoEs).

We discuss what our strategy will be for business development for the remainder of the project. We also give our current thinking on the possible approaches for the sustainability of POP. Finally, we summarise the successes we have made towards our milestones and targets, and our other achievements.

1. Introduction

Business Development for POP is about finding new users of its services. Our strategy is to use a variety of methods, which we discuss in this section. The partners with the most effort in this Work Package are NAG, Teratec and IT4I. Two specific groups were selected for particular attention in the DoA, that is SMEs and our fellow Horizon 2020 CoEs. These were subjects of our earlier deliverables D2.1ⁱ and D2.2ⁱⁱ in which targets and tasks were set.

The three principle partners bring their expertise and partnerships with industry and academia, as well as involvement in other CoEs and European HPC initiatives to the business development activity. As well as the activities discussed in this section, their regular promotional work includes POP. All standard communication channels are exploited including fliers, newsletters, websites and social media. They also take the opportunity to promote POP at many events where a purely POP presence could not be justified.

2. Marketing Activities

In this section we describe the business development marketing activities.

2.1 Target Sectors

POP services are appropriate for any user of HPC and thus the number of sectors is very large. While much of POP business development does not target specific groups, we concentrated some of our efforts on three specific sectors and identified a further two which were more challenging, which we discuss here. This enables us to establish ourselves in each sector and become known to that community, that is, establish the POP brand. Each sector of science and engineering has its own language, so specific marketing materials are required. For some sectors we leveraged our organizational contacts, knowledge, user community awareness and POP “success stories”. However, we did not restrict ourselves to those like materials and engineering but also included others like

bio-sciences and finance which were poorly represented previously. It is worth noting Computer Aided Engineering (CAE) and bio-sciences are two of largest and most dynamically growing HPC sectorsⁱⁱⁱ.

Table 1 shows user sectors of the POP project including all finished and ongoing services since the start of the current POP project.

Table 1: POP User Sectors

User Sector	Number
Engineering	34
Physics	20
Earth and atmospheric sciences	31
Math	5
Biology and genetics	6
Others	17
Total Services	113

2.1.1 Computer Aided Engineering

CAE refers to the use of software tools for engineering modelling, analysis and simulation. This is a broad field and of great importance for European industries, covering finite element analysis, computational fluid dynamics, multibody dynamics, durability and optimization. The community includes academic research and education, as well as the commercial sector, and so has diverse needs and priorities. CAE solutions in turn come in different forms including off-the-shelf software developed by software vendors, in-house codes, engineering simulation as cloud-based services and free tools developed by open-source communities.

CAE is one of the largest and fastest growing HPC sub-sectors. Given the size and diversity of the CAE community, POP needs to identify where its services will be most needed. Big multi-national software vendors such as Ansys and Altair Engineering sit at one end of the spectrum. They produce general purpose CAE tools and have the means to invest in the performance optimization of their software for best use of HPC systems or cloud services. Next, there are CAE solution providers, with a focus on a specific sector of engineering such as automotive, aerospace, chemicals and materials. In these cases, the domain experts developing and maintaining software could benefit from POP expertise in performance optimization. POP2 has several services finished or ongoing for this category of users.

At the other end of the spectrum, many engineers, from SMEs to large firms, rely on in-house codes to deliver their specialised niche analysis tasks. These users often have neither the time nor the essential expertise to invest in the

assessment and optimization of parallel codes. In addition, more and more users, both academic and commercial, are being attracted to use open source solutions such as OpenFOAM. While free and open-source tools encourage collaborative innovation, optimizing the performance of these tools for a customized problem is often a challenging task. Since 2015, there have been more than 10 requests for POP services for OpenFOAM-based codes, with the majority being related to the engineering domain.

The engineering domain accounts for 30% of all POP services. We have explored different avenues to find potential users, including social media (especially LinkedIn groups), presence at events and conferences, prior contacts and professional bodies.

CAE is a big community and given that POP only started in 2015, our marketing messages can easily get lost without reaching potential users. To bring our business development cost down, we need to establish ourselves in the community. This understandably takes some time and requires good understanding of the sector, well-thought-out marketing strategies and forming business relationships with key companies and associations. One avenue we are exploring is to establish relationships with leading engineering associations. We have already had some success with NAFEMS: the International Association for the Engineering Modelling, Analysis and Simulation Community (for details see section 2.6) as well as research centres such as CERFACS^{iv}, CEA^v and CNRS^{vi}. This will help us not only to increase our reach but also to understand our users' needs better.

For the second half of the project, we will continue to work with NAFEMS and identify other professional associations and innovation hubs that can help us spread the word about the POP project and its services. Closer collaboration with software communities, free or commercial, such as OpenFOAM and SimScale is another avenue that we will explore. We will continue our collaboration with the EXCELLERAT CoE, which focuses on engineering applications, particularly aeronautics and the automotive industry, and has set goals to reach exascale performance for six reference applications.

2.1.2 Biology and Life Sciences

Biology and life sciences is a hugely diverse field which is continuing to grow in its use of HPC for both traditional and an explosion of new computational methods. Examples of areas in the sector with heavy use of HPC include in silico drug discovery, which makes use of molecular dynamics, docking and protein folding simulation, often combined with deep learning for target discovery; biomechanics, which makes heavy use of finite-element modelling to model skeletal structures and supporting tissues; and systems modelling using multi-physics approaches to model complex biological systems involving interactions with e.g. fluid dynamics, finite element and agent-based models to simulate blood flow within the human vascular system.

The software landscape within the biology and life sciences sector is, however, dominated by a small number of widely used commercial and open source packages. These are typically not biology specific applications, and overlap strongly with physical and quantum chemistry, CAE and materials modelling. This means that software development within the sector is more commonly scripting work intended to allow use of these established packages in custom workflows rather than development of custom HPC applications. Some of these well used packages, such as OpenFOAM, have already benefitted from POP assessments and proof-of-concept work, and having gained an understanding of the packages used within the sector, we can make more effective use of these success stories to improve the marketing and publicity materials which target the sector.

The CompBioMed CoE is an important project in the biology and life science sector, and we have a successful ongoing collaboration with CompBioMed started in the POP1 project to optimise their flagship HemeLB exascale vascular modelling application (see section 3.1).

As a result of what we have learned in the first half of the project, an effective approach for POP is to identify the packages that are commonly used and try to engage with the developers of these applications directly. In addition, we can use the success story of HemeLB, along with OpenFOAM, to develop more relevant marketing material for use in the bio-sciences sector.

2.1.3 Computational Materials Science

The materials science and engineering sector widely utilises modelling and simulation to discover stronger, more durable and lighter materials for a wide variety of purposes, such as aerofoils and car chassis. Materials science is an interdisciplinary field incorporating elements of physics, chemistry and engineering. Simulation in this sector is done across a range of different length and time scales:

- Quantum level: based on Density Functional Theory
- Atomistic: molecular dynamics
- Coarse-grained: using scale-bridging techniques, e.g. a simulation could use a hybrid of quantum mechanics and molecular dynamics
- Meso-scale: using methods such as Dislocation Dynamics and the Phase Field method
- Continuum scale: using continuum mechanics and finite element simulations.

There are a large number of academic and commercial codes used for materials science simulations. Based on empirical evidence, research software such as VASP scales up to hundreds of processes, whereas commercial codes don't scale as well. Thus, the commercial sector, including SMEs, can potentially benefit from the POP service.

The materials science sector can benefit from better scaling to tackle more challenging problems. One of the trends in materials science is data sharing with collaborators, and there is a huge investment in this area. Whether this provides further opportunities for POP remains to be seen. Nevertheless, given the range of simulation tools used and the importance of good performance, there is a lot of potential for attracting new POP users from this sector.

The European Materials Modelling Council (EMMC) is an innovation hub with access to a large number of SMEs in Europe. They provide a great channel to promote POP within computational material science and have advertised POP via their twitter account. We plan to continue our conversation with them for further dissemination activities. Besides, we plan to attend materials science events such as the EMMC International Workshop 2021^{vii} to promote POP, learn more about the sector and identify the user groups or software packages in the sector that can benefit most from POP services.

2.1.4 Finance and Insurance

One of the more challenging sectors is Finance. Market segmentation for financial services reveals many disparate domains, e.g. accounting, banks, brokers, proprietary trading outfits, hedge funds, financial market participants, risk management and trade idea generation. The problem is that these domains have very little in common. This is very different to other sectors such as CAE where there is much more commonality, e.g. a small set of equations can be used to model a wide range of physical systems. The disparity in the finance sector is an obstacle for POP business development given our limited resources. It is also highly unlikely for finance firms to grant us access to their software, which in turn would make it more difficult to generate success stories and marketing materials. The efforts in this sector have mainly involved the attendance of events where a POP partner had an interest outside of POP, and unsolicited mailing.

2.1.5 High Performance Data Analytics and Machine Learning

These fields represent another difficult sector. Both have been rapidly evolving in recent years, and the rate of change is reflected in their software landscape. There are a range of notable software frameworks and libraries that are well optimized for their intended workflows and can be used with scripting languages such as Python. The differences between objectives and top-level characteristics of these applications and the traditional HPC workloads have led to the development and use of different workflow and software tools in these domains. However, their common ground is the need to process large amounts of data and there is a clear trend towards innovative approaches that will create significant value by bridging the gap between these technologies and HPC, e.g. scaling up deep learning trainings across nodes and blending traditional HPC simulation with deep learning techniques.

Most traditional HPC applications are written in Fortran or C/C++ with MPI and/or OpenMP parallelism. While the POP performance assessment tools

were developed with a focus on classical HPC applications, we have extended our services, methodology and tools to support most parallel codes, including Python and CUDA applications. This service-oriented approach allows us to learn and cover the emerging needs in combined simulation and data analytics applications. Given that we still need to learn how and if our services could be tailored for HPDA and machine learning users, we cannot focus our limited business development resources on these sectors yet. Instead, we will watch developments in these domains and actively look for new users, especially via social networks and by unsolicited contact.

2.2 Unsolicited Marketing

Potential POP users are researched using a variety of digital means including internet searches; the websites of conferences, codes and HPC centres; and LinkedIn. Initially, an email is sent giving details of the services POP offers, tailored to the lead as much as possible. This can be followed up by further emails or telephone calls. All interactions with potential users are recorded in a Customer Relation Management system. This activity is very time consuming and therefore expensive. At the end of this section we take a look at the sources of leads.

Working with Focus CoE as part of their WP3 “Industrial Relations” activity, 41 companies were identified and sent POP information. So far, none of these leads have become POP users. As we will discuss later, however, this is below the number of leads we generally require to generate a single POP user.

2.3 Events

Events are a very attractive activity, as they offer an opportunity to talk directly with potential POP users. However, it is difficult to gauge how many users have come to POP as a direct result of talking to a partner at an event. Below we look at some of the significant events we have attended.

In 2019, we went back to the International CAE conference in Vicenza, Italy. POP had a booth as part of the “Research Agora”. This is a well-attended event with a huge presence from the industry. The 2019 CAE Conference and Exhibition attracted around 1,500 delegates and over 70 exhibitors and sponsors from different industry sectors. A successful outcome of this event was getting an article about POP published in the EnginSoft newsletter. A downside of busy events such as this is the difficulty of standing out among the huge number of other exhibitors, especially when we are not yet established as a brand in the community.

POP joined the CompBioMed and Focus COEs in attending BioFIT 2019 in Marseille. We had a shared booth where we were able to present the contributions of the CoEs and discuss potential collaborations with the attendees who visited our booth. BioFIT attracts a wide range of attendees from both science and industry, working on innovative projects in drug discovery, genomics, medical imaging and bioinformatics. The event was a success in terms of lead generation, providing sixteen new business leads and contacts

with five professional bodies. However, subsequent detailed interaction with these leads revealed that although all the leads were using parallel HPC, they were using existing off-the-shelf HPC software and their development was limited to scripting and orchestration of these packages into their desired workflows. Nevertheless, attending this event was extremely helpful in building a much better understanding of the biology and life sciences sector.

The Teratec Forum is an annual event held in France which brings together international experts in HPC, Simulation and Big Data. In 2019, this event welcomed more than 1,300 attendees. With a diverse range of talks, workshop and exhibitors, this event highlights the technological and industrial dynamism of the HPC sector and creates an atmosphere most suitable for POP marketing and dissemination activities. At Teratec Forum 2019, Focus CoE organized a joint booth serving as an information hub for HPC CoEs. POP, along with EXCELLERAT and HiDALGO, presented their work on posters and through booth presentations. Experts from the four CoEs were present at the booth and engaged in many discussions with interested forum attendees.

IT4I participate in significant HPC-related events, especially in the Czech Republic, Poland, the Slovak Republic and Austria. HPC user meetings such as the IT4I user conference and Austrian HPC Meetings have proven fruitful in terms of acquiring POP users.

See Table 8 in Appendix 8.1 for a full list of events attended. We had a target to attend six sectoral events, which we have surpassed.

Besides, we have organized training events for our potential users and sponsored tutorials and workshops in cooperation with other HPC initiatives. For more details see POP Deliverable D4.1^{viii}.

2.4 Marketing Materials

The project has created various marketing materials. Appendix 8.3.1 shows the artwork for a “pop-up banner” to take to events. We put a lot of effort into producing a “glossy” brochure. Some example pages are shown in Appendix 8.3.2.

We produced several fliers. As well as an update to a general one, we produced three targeted at specific sectors. Appendix 8.3.3 shows an example of one of these. We also produced a flier for energy efficiency, shown in Appendix 8.3.4, which was a target in D2.1.

2.5 External Publications

We publish important POP news and results in various external channels maintained by either our collaborators and customers or general HPC news sites. We have provided content or published articles in our fellow CoEs’ newsletters including Focus CoE, CompBioMed and E-Cam (for details see section 3.1). In addition, we published articles at EnginSoft, Intel Parallel

Universe magazine and Inside HPC online news (for more details see POP Deliverable D4.1).

2.6 Professional Bodies

Advertising POP services through professional bodies, like trade bodies and special interest groups, is attractive as it means we can potentially reach a large audience through a single contact. These organizations have mailing lists, newsletters, etc. that we can exploit. However, getting responses has proved challenging unless we have a personal contact there. We had a target of contacting 20 professional bodies, which we have surpassed.

An example of a successful interaction with a professional body is our contact with NAFEMS, the International Association for the Engineering Modelling, Analysis and Simulation Community. NAFEMS is a non-for-profit organization established in 1983. POP had attended NAFEMS UK conference in 2016. In 2019, we approached NAFEMS. As a result, POP has been advertised in NAFEMS CFD working group mailing list, and we have been offered the opportunity of publishing an article about POP in NAFEMS quarterly magazine with about 100k readers. We will be present at NAFEMS UK conference 2020 as an exhibitor. In addition, our talk titled "*Parallel Engineering Codes: Performance Optimisation with POP Methodology*" has been accepted for presentation at the same event. Our proposal for a NAFEMS Webinar titled "*How to understand and improve the performance of your parallel applications*" is under review. Being present at events, giving talks and webinars and having articles in newsletters and magazines are complementary activities that help establish the POP brand in the community.

See Table 9 in Appendix 8.2 for a list of the professional bodies we have contacted.

2.7 Social Media

Specifically, this refers to the use of LinkedIn and Twitter. LinkedIn has mainly been used to source leads and Twitter for the marketing of the POP service, although this division is not a strict one.

2.7.1 LinkedIn

The two main approaches to finding leads using LinkedIn are networking and searching. They are both ultimately ways of finding companies, and the appropriate contacts within them, who have an HPC code and are a candidate for an assessment. First of all, the networking approach involves joining groups whose members might run HPC codes, following appropriate hashtags and following individuals active in a field of interest. These groups and hashtags could be very general to HPC or specific to certain types of computation or field. For example, the most productive three groups in our experience have been the Computational Fluid Dynamics Group, PRACE^{ix} and the European Materials Modelling Council. Useful hashtags include #CFD and

#simulationsoftware. The benefit of this networking approach is that interesting leads often appear in the user's feed. One particularly good example of this being that SMEs often advertise within these groups. It is then fairly straightforward on LinkedIn to investigate that company further, as well as their employees and skills.

The second approach on LinkedIn is to directly use its search facility. This is useful but not always very efficient in terms of lead generation in a given time. Various filters can be applied to refine the search and then interesting companies can be followed and researched to find the best contact. There is a nice feature whereby LinkedIn informs you who else has viewed a particular company, which can provide further leads. There is also a paid option called "Sales Nav", which allows you to create searches and then get updated daily with new contacts, as well as getting updates from companies that you follow, with such things as jobs changes or new employees.

2.7.2 Twitter

The role of twitter is a combination of both business development and dissemination. In terms of the former, we often directly tweet about who POP is and what services we offer. We also tweet about our success stories, as evidence of our expertise, and to advertise our webinars, which increases our contacts through registrations. Finally, we use more general tweets to raise our profile within the HPC and other sector-specific communities.

It should be noted that twitter can potentially provide leads and LinkedIn is also used to more directly promote POP but the platforms are generally more suited to the uses described here. It should also be noted that to maintain a presence and community engagement on social media requires a non-trivial investment of time.

2.8 Webinars, *POPCasts* and Other Online Content

Webinars have a dual role in providing both dissemination and business development opportunities. The main benefits for the latter are the increased visibility of the POP brand and the demonstration it provides of POP's expertise. In the previous POP project, all webinar attendees were e-mailed individually with personalised e-mails about how they could benefit from POP but they only rarely became users of the service. The current strategy is to select only the most promising leads to send such targeted e-mails. D4.1 reviews our online content including webinars in more details.

A task from D2.1 was to produce three on-demand short webinars aimed at managers in SMEs. After exploring the various ways we could approach this, we hit upon the idea of recording interviews with POP staff and users. This has the advantage that they are conversational and don't require high production values or polished voice overs. We call these short videos *POPCasts*! We have interviewed a POP Business Development Manager, a user and a POP Analyst. These *POPCasts* were released every other week starting on April 28, 2020. The number of views is staggering with the first one receiving over 120 views

in only four weeks and second one receiving 49 views in two weeks. We think this is very promising.

Other online content like blogs and newsletters help drive POP business, although are primarily a dissemination activity and so are discussed in D4.1.

Another digital business development activity we are pursuing is online training.

2.9 Training as Business Development

We have created an online training “portal” which is in the early stages of development. We gave ourselves this target as part of our targeting of SMEs. It has the dual function of providing useful information to users and attracting potential new users. The hope is the pages will be linked to from external sources and visitors will be inclined to read more about POP.

The portal includes a collection of self-study modules which are being developed in cooperation with Work Package 4. Each module includes a training video and has a page with further reading materials and links to other POP resources to give a “joined up” approach. We will monitor the number of visitors to the site, and any feedback we get, and consider if the training offering should be expanded.

2.10 Material for SMEs

Our first deliverable was concerned with targeting SMEs and our tasks and targets are given in Sections 6.2.1 and 6.2.2 respectively. However, after additional consideration we realised we could produce material that spoke to SMEs and non-SMEs alike. This material was discussed in Section 2.4.

We have also produced blog posts aimed at SMEs in line with our targets. We are investigating further ways we can provide website material targeting SMEs, including specific landing pages. Currently we can give potential users a special URL which takes them to our SME focussed blogs.^{xi}

How to provide SME training at events is still an open question. We are considering making this an online activity and are waiting to measure the impact of our POPcasts and online training materials before we progress this further. Indeed, the online training portal may also fulfil this target.

2.11 Sources of POP Users

After 18 months we have almost 1000 leads. This has converted to 93 new users, four of which decided not to complete the service. Users “drop out” for a variety of reasons, including resource issues. This represents a conversion rate of 8%, i.e. you need 12 leads to get one user. If we single out SMEs we see that we need 33 leads to achieve one new POP user. This is because half the leads are SME leads and we have 15 SME users, a conversion rate of 3%. In D2.1 we set a target of 280 new SME leads, which we have exceeded.

It is tempting to look at the above conversion rates and draw conclusions on how many leads we require to hit our KPIs. However, they do not tell the full story. Table 2 shows the source of the leads for the 89 POP users.

Table 2: Source of POP Users

Source of User	Number
Previous Contact of POP Partner	25
Local user of POP Partner	9
Existing POP User	5
Business Development	20
Word of Mouth (Non-POP Marketing)	8
Source of Lead Unknown	14
ChEESE Cyclic CoE Campaign	8
Total	89

From this we see that only around 20% users were found as a result of business development work, ignoring the unknowns. Thus, of our 1000 leads the conversion rate is about 2%, we need nearly 50 leads to get a single POP user. Two thirds of users found through business development were from the engineering sector.

Only one SME dropped out, a rate of only 8%. Our drop out rate is much lower than the first POP project.

2.12 The POP Brand

All of our activities promote the brand. The POP metrics, methodologies and our services have to be seen as best practice if we are to continue to succeed.

3. Collaborations

3.1 CoE Collaborations

All EU-funded CoEs for computing applications aim to strengthen Europe's leadership in HPC applications. POP provides services across all domains of science and technology while the other CoEs serve specific disciplines. Their work involves improving scalability of HPC applications (especially towards peta and exascale computing), improving the usability of major existing software packages, devising new workflows where needed and building competence among user communities through training programs and promotion of best practices.

POP expertise in performance optimization and best practices along with the domain expertise of the other CoEs creates synergy for the advancement of HPC software ecosystems in all domains. In D2.2, we described our strategy for targeting other CoEs and set ourselves six tasks to build collaborative relationships with the other CoEs (for details, see section 6.3.1). We have completed all these tasks.

We have established a network with other CoEs with a single point of contact at POP (see Table 3). With the help of this network, all CoEs have been invited to collaborate with POP and they are aware of possible avenues for collaboration.

Table 3: CoEs, the POP Partners involved and our Point of Contact

CoE Name	POP Partners also in this CoE	Point of Contact
BioExcel	BSC & JSC	BSC
ChEESE	BSC & HLRS	BSC
CompBioMed	BSC	BSC
E-CAM	JSC	JSC
EoCoE	BSC, JSC, RWTH Aachen & UVSQ	BSC & JSC
ESiWACE	BSC	JSC & BSC
EXCELLERAT	BSC, HLRS, RWTH Aachen & Teratec	HLRS
HiDALGO	HLRS	HLRS
MaX	BSC & JSC	BSC
Focus CoE	BSC, HLRS, JSC & TERATEC	BSC, NAG & JSC

Our established network with the CoEs allows effective and regular communication, helps maintain the relationship with the CoEs and ensures all possible collaborations are exploited. For example, this network undertakes our formal periodic campaigns as set out in WP5 Task 5.3. Table 4 lists the performance assessment services undertaken for other CoEs; so far, POP has undertaken 11 services for ChEESE, 2 for EXCELLERAT, 2 for CompBioMed, 1 for EoCoE and 1 for EsiWACE. The CoEs continue to develop new functionalities for their flagship codes. We expect to provide further performance assessment services for CompBioMed, E-CAM, EoCoE and ESiWACE2 when new versions of their codes are ready for assessment.

This network has also proven highly effective for identifying events where attendance is beneficial, as well as organizing joint workshops or training

events for European HPC initiatives which include the other CoEs. Table 5 lists the training events with confirmed details. The discussion about future events is currently suspended due to the Covid-19 outbreak. The network will resume planning of joint events as soon as there is enough information to decide the best course of action.

Table 4: Performance assessments for CoEs

Code Name	EU Project Name	Number of Assessments	POP Partner in charge of the work
FALL3D	ChEESE	1	BSC
Salvus	ChEESE	2	JSC
SeisSol	ChEESE	2	JSC
Specfem3D	ChEESE	1	JSC
ExaHyPE	ChEESE	1	HLRS
ASHEE	ChEESE	1	HLRS
PARODY_PDAF	ChEESE	1	NAG
Tsunami-HySEA	ChEESE	1	BSC
xshells	ChEESE	1	NAG
1D-NEGF	EoCoE	1	JSC
Alya	EXCELLERAT	1	BSC
AVBP	EXCELLERAT	1	UVSQ
HemeLB	CompBioMed	1	JSC
DeaLAMMPS	CompBioMed	1	BSC
IFS-ST and IFS-FVM	EsiWACE	1	BSC

Finally, this network helps POP to engage with the other CoEs in a range of dissemination and outreach activities including newsletters, webinars, conference talks and joint presence in events. Examples are:

- POP webinar series: We invite presenters from the other CoEs for the POP webinar series. In Nov 2019, Claudia Rosas and Mauricio Hanzich, working for ChEESE, gave a webinar titled *“The Successful Interaction of ChEESE and POP - a cross-collaboration of CoEs”*. In May 2020, Jon McCullough, working in CompBioMed, will give a webinar titled *“CompBioMed CoE - Addressing Biomedical Challenges with High Performance Computing”*.
- Newsletters: Focus CoE published an introductory article in the September issue of their newsletter, and an overview of recent POP activities will be published in their May issue. E-Cam will promote POP in their next

newsletter issue, including an overview of POP services and a domain related success story.

- POP attended CompBioMed Conference 2019. Craig Lucas from POP gave a talk titled “The POP Centre of Excellence - Improving Parallel Codes”.
- POP and CompBioMed attended BioFIT 2019 and jointly ran a booth, coordinated by FocusCoE. This joint attendance was a successful exercise; CompBioMed’s knowledge of the domain complemented POP expertise in parallel performance best practices well, allowing more effective communication with the conference attendees.

Table 5: CoE Training Events

Training Activity	EU Project Name	POP Partner(s)	Date of Activity
Workshop	E-CAM	BSC & JSC	8-10 Jan 2019
Workshop	E-CAM	JSC	6 Jun 2019
Workshop	EoCoE	BSC & JSC	16-20 Sep 2019
Workshop	EoCoE	BSC	7-10 Oct 2019
Workshop	EoCoE	BSC & JSC	Postponed due to Covid-19
Workshop	VI-HPS	JSC	Postponed due to Covid-19
Workshop	VI-HPS	BSC, JSC & UVSQ	Postponed due to Covid-19

Clearly, our collaboration with some CoEs is further developed than with others. Our experience shows that each joint activity leads to further collaborations; POP services are essential for advancement of HPC applications and a CoEs’ domain knowledge is invaluable for POP. Our collaboration with CompBioMed is well-established and has produced useful marketing materials including success stories from multiple iterations of performance assessments and improvements for the HemeLB code, a flier produced for our joint attendance at BioFIT 2019 and a future POP webinar. This is especially helpful for our business development activities in the biology and life science sector. To help our sectoral business development activities, we will pursue further collaboration opportunities with other CoEs especially EXCELLERAT, CompBioMed and BioExcel.

3.2 HPC Centres

We are developing collaborations with local/national HPC centres in Europe. So far, we have established a relationship with two centres:

3.2.1 SURFsara

SURFsara, the Dutch National High Performance Computing centre, first offered to advertise POP within their user community and then identify user codes running on their machines which could benefit from POP services. One POP assessment has already started. They would like their analysts to be actively involved in the performance assessment services with the goal of eventually being able to do the assessments themselves. They have also expressed interest in a one-day POP training workshop.

3.2.2 ICHEC

ICHEC, the national HPC centre in Ireland, are keen to use our methodology, which is a great endorsement of our approach. They offered to advertise POP within their user groups and are interested in receiving training materials from POP about the POP methodology and tools. They want to teach these materials themselves, as they have KPIs in this area. They are interested in POP services where their analysts are involved in the process and ultimately, they want to do the performance assessments themselves which is a form of sustainability. They are a EuroHPC Competence Centre.

3.2.3 Interaction

With this type- of close collaboration, POP is helping HPC centres to build and sustain a pool of skilled HPC experts. This strengthens the local HPC ecosystems and is especially important in European countries where HPC is not well established. At the same time, these centres will help us to spread the word about the POP methodology and the POP services in their local community. These centres embracing the POP methodology is a big step toward POP sustainability.

4. Business Development Strategy for the Remainder of the Project

4.1 Events

We will continue to attend events, concentrating on our chosen sectors and exploiting opportunities at any events where a POP partner is present but POP is not the primary focus. We will continue to engage with Focus CoE and their coordinated events.

4.2 Marketing Materials

We have created a large collection of materials so do not envisage expanding this greatly. We will exploit the templates we have created and generate more fliers targeting particular audiences.

We are currently working on a T-shirt design for an engaging giveaway at future events. They should attract people to a booth at a conference or exhibition, allowing us to have that first, and vital, conversation about POP.

4.3 Professional Bodies

We will continue to engage with professional bodies but will look at better ways to do this. We will use our experience with NAFEMS as a guide.

4.4 Independent Software Vendors

We have followed several ISV leads from large industrial, to SMEs and academia. We have had mixed responses. For example, Altair Engineering France has declined the invitation to use the POP services. This is not surprising as discussed in section 2.1.1. So far, we have four users who sell their applications, two from academia and two SMEs. This target group will receive particular attention in the second half of the project.

4.5 Online Content

We will monitor the impact of our online training, webinars and *POPCasts*, by keeping track of the viewing figures.

4.6 Cloud Providers and Integrators

In our first deliverable we set ourselves a goal to investigate the potential of strategic partnerships with at least one each of HPC vendors, integrators and cloud providers. While they are not likely to be using POP services, their customers are. The challenge here is to find partners that are not looking for direct and short-term benefits from POP services. For example, there have been potential partners where their interest lay outside of our remit. On the other hand, we have recently formed a relationship with BIOS-IT^{xii}. They are interested in the POP services and not for their own benefits but for their customers. They have offered to spread the word about POP among their customers and contacts. We will monitor the outcome of this relationship in the coming months and look for other potential partners as we think there is a real opportunity here.

4.7 More Collaborations

Identifying strategic collaborators and forming business relationship with them is a core part of business development. We have been successful in this regard, setting strong relationships with most of our fellow HPC CoEs and a couple of HPC centres. Building on our experience, in the second 18 months, we will explore other avenues of collaborations including academia, EuroHPC Competence Centres and Innovation hubs.

We will explore ways to promote POP and its methodology to people who are about to learn about HPC, i.e. the next generation of HPC users and HPC experts. Universities are the best platform to reach these groups. For example, this includes university students taking related modules at computer science departments, PhD students working in computational science and early career researchers who need more advanced computation to carry on their research. Universities provides the best platform to reach the next generation of users and experts. NAG is well connected to the academic sector and universities,

especially in the UK. We have made an academic flier and plan to approach our contacts in universities and research and associated bodies such as the RSE network^{xiii}.

IT4I just became a member of the EuroHPC Centre of Competence network. This network, with more than 30 partners from all EuroHPC member states, is a great channel for promoting POP services. IT4I plans to promote POP within its Centre of Competence activities including training courses, workshops for HPC industrial users and specialized solutions for industrial partners.

IT4I also plans to promote POP services via networks of Digital Innovation Hubs (DIHs) at regional, national and European levels. IT4I and Moravian-Silesian Innovation Center have established Digital Innovation Hub Ostrava^{xiv}, aiming to help SMEs in the Moravian-Silesian region with the adoption of HPC technologies in their businesses. CEEInno platform coordinates all DIHs and organizations focused on digital innovations in the Czech Republic. Finally, all DIHs in Europe and their networking activities will be coordinated and financially supported within the Digital Europe programme. IT4I plans to target SMEs using all these channels.

4.7.1 Open Source Community

Some open source projects have become the *de facto* tools for computational tasks in their relevant domains of science and engineering. These projects with a big community of users play a central role in education, research and innovation and their use in HPC applications is becoming more widespread. While some of these projects have been very successful in building a collaborative community of innovators, they are usually not optimized for best performance especially on HPC systems. POP can have a great impact by helping these communities to improve the performance of their code. For example, POP has already undertaken eleven performance assessments for OpenFOAM-based codes. To increase our visibility in these communities, one approach is to identify the packages that are commonly used in HPC applications and try to engage with their developers directly. To start this model of collaboration, OpenFOAM is an obvious candidate.

4.8 Further Analysis

We will work to increase our understanding of the business development process and where leads come from. We will look at the effectiveness of working with external sites, like those we have set up in collaboration with, and the existing and future HPC communities, including PRACE and EuroHPC Competence Centres. This analysis and the results of future Return on Investment information from WP3 is vital in being effective going forward and in beginning to understand how the POP service can be sustained into the future.

5. Sustainability

In this section we look at the sustainability of POP.

5.1 Improvements Made in the Project

Throughout the business development activity in this project we have sought to lower our operational costs. Whilst much work is needed to find, contact and follow up leads there have been other activities which are more cost effective. This includes making templates for fliers; contacting professional bodies who in turn can publicise POP to a large number of people; working with HPC Centres to promote the POP methodology; and hosting a range of online materials, like the POPcasts, webinars and training materials, that can be viewed on demand. We have also narrowed our focus to certain sectors so we can concentrate on reaching them on multiple fronts.

If the tools are easier to install and use, it is natural to ask if the time to perform a POP Performance Assessment is reduced as a result. To get insight, we have started recording the breakdown of time for Performance Assessment services covering installation time for the tools and user application; the time to trace and analyse the code with the POP tools; and the time to write the report for the user.

Table 6 shows the breakdown of time for an indicative subset of assessments and explanatory comments. It is clear the figures vary enormously, and it is impossible to draw a conclusion at this point. However, as the project continues, we hope to see a reduction in the overall time to produce an assessment. Thus, whichever route we take in the future, it would be cheaper to provide this service.

5.2 Sustainability Options

In this section we outline the current thinking for options we have for making POP sustainable. These will be explored in detail over the coming months, or expedited should an appropriate funding call be announced. As part of this process, we will look at what could immediately follow the current project and what a long term solution to sustainability could be. A key aspect to solve is what services we can charge for, and who would be likely to pay for them.

Several factors need to be taken into account from the successes of the first two POP projects, to interfacing with current and emerging HPC initiatives like EuroHPC Competence Centres.

One option we have ruled out is to spin off an entirely commercial enterprise. This is not attractive to most academic partners, and for some their participation would be prohibited by their constitution. The POP service is the application of research, providing a service to the community while having a test bed for tools and an opportunity to learn about the parallel paradigms used in HPC codes, which are poorly supported by commercial tools. It complements the

development of programming languages and systems and their other academic work. It also provides a valuable training ground for analysts who leave academia and move into industry.

All options need the continuation of the establishment of the POP brand, an activity which requires more time than that for which POP has operated to date. We also need universal buy-in to our methodology, which is our unique contribution to the community. It needs to be recognised and valued. IT4I, and other collaborators, are embedding POP processes into their “business as usual” activities. This is a form of sustainability and will complement any approach we ultimately pursue.

Table 6: Time Breakdown (in hours) for a Subset of Performance Assessments

Install Application	Install Tools	Trace	Analyse	Write Report	Total	Comments
12	0	24	30	2	68	Follow on assessment with custom analysis
1	0	1	3	3	8	Follow on assessment (Mainly comparing scalability and POP Metrics)
19	11	48	55	34	167	Multiple tools used, Problems in trace collection, and using tools
1	4	24	16	12	57	Ran smoothly
9	3	42	97	50	201	Complex applications, Problems using (multiple) tools
6	1	6	6	5	24	Ran smoothly
2	72	4	24	24	126	Helping customers to set up test cases and traces
2	0	48	16	24	90	Ran smoothly
7	0	15	67	29	118	Multiple tools used, complex application behavior
1	16	24	40	16	97	Issues with tracing led to more analysis work
2	40	8	40	16	106	Multiple tools used
6	1	16	16	4	43	Ran smoothly

What follows the current project is crucial for the POP sustainability. We have identified three options to support the continuation of the POP consortium. We will explore the viability of these options over the coming months. The rest of this section provides an overview of each option and their pros and cons.

5.2.1 Fully Funded Under EU Research and Innovation Programme

We will consider the value of POP to the HPC community including users, service providers, and other HPC initiatives and decide whether the best investment is to guarantee continuity of POP in its current form with a third round of funding, should it be made available. Currently, the POP CoE supports the other HPC CoEs and EuroHPC Competence Centres by providing them services that are essential to their success but are not defined as their core activities. The future of all Horizon 2020 Centres of Excellence is currently being considered. When the outcome is known we will have a better idea how to position ourselves in the new European HPC landscape.

Given the improvements made in the project, discussed above, and the establishment of collaborations and the POP brand, we may require less financial support to deliver the same service.

Pros

- Continuation of all POP services for the community.
- We can further develop existing and new collaborations.
- Business development will be fully funded.
- Continuity in building a pool of experts in HPC performance by training analysts and users and job security for current POP analysts.
- We can continue to prepare the community for exascale.
- We can continue to help SMEs maximise their use of HPC.
- Enough time to test and establish the new metrics and methodology that are under development in POP with non-traditional architectures and HPC applications in non-traditional domains.

Cons

- There would still be a significant cost to the EU.
- It could be a complicated model if some users pay for services.
- Long term sustainability is no clearer.

5.2.2 No Structured Funding

This would be a loose consortium continuing on a best effort basis. We could position ourselves as the custodian of the POP methodology and the subset of partners participating in that activity could acquire funding through traditional routes for academic research. There would need to be a mechanism for input from the community. Similar input would be required to the tool developers who would also need to seek funding to continue their development.

We could consider a membership scheme to which HPC centres could subscribe. There would need to be some quality control to ensure the POP methodology is followed. For example, we could have a scheme for training and accreditation of a member site, or individual analyst. We would connect potential users with centres that could provide free services, where appropriate, or to commercial entities who can carry out Proof-of-Concepts, for example, on a paid consultancy basis. This model, of POP being a broker for this type of services, might be satisfactory to a large group of our customers; in a user

survey, given in D3.2^{xv}, nineteen out of thirty-five POP2 users expressed interest in a Proof-of-Concept service.

Under this model we need to consider which activities need to continue and how to support them. We need to maintain the POP website and mailing lists. We need to decide what marketing strategies can be undertaken with little resources, like the newsletter and webinars. We need to find alternative platforms to deliver training on the POP methodology and metrics. One possible option is to provide training in collaboration with VI-HPS^{xvi}. Collaborations would be essential to the success of this model. We would need to fully integrate with the Competence Centres, the Horizon 2020 CoEs and other future HPC initiatives under Horizon Europe Programme.

It will be important to reduce the cost of services. Automatic analysis will be really error prone, an expert is required to look at data. However, it is possible to automate part of the process, e.g. the POP metric calculations. Some of our tool development efforts especially PyPOP^{xvii}, as well as improvement in Cubex^{xviii} and BASIC ANALYSIS^{xix}, have helped reduce the burden on POP experts. Building further on this, some automatic assessment of user code might be possible. Perhaps the tools could give a “seal of approval”, that is, confirm the POP metrics are all greater than 80%, which indicates reasonably good performance for parallel applications.

Pros

- Member sites would be engaged in a wide POP community.
- There would be synthesis with Digital Innovation Hubs. IT4I plan to integrate POP services into those offered by their hub.
- There would be synthesis with EuroHPC Competence Centres.
- A scheme of partner or personal accreditation could be attractive to members and users.
- Services offered can be tailored around customer needs and budget, not constrained by project deliverables.
- Many services would need to be charged for.

Cons

- Reduced POP services for the community, including metric and tool development.
- Tool developers would be less obligated to incorporate POP metrics in their software.
- Training and mentoring would need to be provided to member sites,
- Reduced support to the community for progression to exascale.
- There would be no free support for SMEs.
- Free support for academic users depends on availability of other funding and is not guaranteed.
- Lacks buy-in from the EU.
- Reduced business development and marketing activities might lead to the POP brand not surviving.

5.2.3 The Middle Ground

The third option is to support the continuity of POP under public funds but with a smaller budget, possibility EU "Core Support Action" funding. This will allow POP to provide some core services. We could offer, perhaps, free Performance Assessments, and we would be able to maintain the support functions of business development, customer advocacy and training.

We will investigate a host of ways that our technical services can be offered or provided by other means. Individual services for academic users can be funded through research grants by requesting money to pay for POP services or the staff that would provide them. This sustainability option would have a membership, like that described above.

Commercial users of POP could access services through PRACE or pay those POP partners that are able to accept payment for services. A basic POP Performance Assessment could be a "pre-sales" activity, that is provided for free to entice users to pay for a more detailed study or Proof-of-Concept. The latter could fund the former, although they would have to be underwritten in advance. Similar to the second option, there would be more flexibility to tailor services according to customer needs and budget. Also, new services could be offered, for example a "Seal of approval" given by POP for customers who want to run their code on European HPC facilities and have to justify their code meets the performance requirements.

Some POP partners have other sources of funding for doing similar services to POP. Care would need to be taken to integrate these in a cost-effective way that does not detract from either project or its KPIs.

Pros

- Member sites would be engaged in a wide POP community.
- There would be synthesis with Digital Innovation Hubs. IT4I plan to integrate POP services into those offered by their hub.
- There would be synthesis with EuroHPC Competence Centres.
- A core service of free Performance Assessments to academic users could be guaranteed.
- We could leverage existing collaborations.
- Training and mentoring could be provided to member sites.
- The maintenance of the POP brand could be achieved, particularly in sectoral user communities.
- Services offered can be more tailored around customer needs and budget.

Cons

- POP would still be dependent on short-term funding.
- There would be no free support for SMEs.
- No guaranteed level of support to the community for progression to exascale.
- The future of non-core services such as co-design activities is uncertain.

- Less budget for research and development could impact extending/testing the POP methodology for emerging applications in non-traditional HPC domains.
- Some services would need to be paid for.

6. Results and Impacts

In this section we consider our milestones, targets and tasks from earlier deliverables and our other successes.

6.1 POP's Milestones

The relevant milestones for this document are given in Table 7.

Table 7: POP KPIs Related to Business Development

POP Milestone	Month to Achieve by	Result
50 POP Users	12	75 POP Users, KPI met
90 POP Users	24	On target to reach KPI, currently 89
10 POP SME Users	12	11 SME POP Users, KPI met
20 POP SME Users	24	On target to reach KPI, currently 15

6.2 D2.2 Plan for Targeting SMEs

This deliverable outlined how POP planned to identify and attract SMEs as customers of its services. We identified the methods we would use to research the market, locate possible SME users and described the material we would produce to target them.

6.2.1 Tasks

In order to achieve traction within SMEs we set ourselves the following tasks:

- Update the POP website with specialist material aimed at SMEs.
- Attend 6 sectoral events in the first 15 months of the project.
- Identify and contact 20 professional bodies spanning the entire EU by month 12 of the project.
- Investigate the potential of strategic partnerships with at least one each of HPC vendors, integrators and cloud providers.
- Produce marketing material aimed at code developers working in specific sectors to include at least Oil & Gas, Pharma and CAE.
- Produce marketing material aimed at managers in sectors to include at least Oil & Gas, Pharma and CAE.
- Produce marketing material to highlight the new energy saving profiling which will be introduced by POP2.

- Investigate what print and digital media would provide cost-effective advertising for POP.
- Investigate opportunities for SME training at events.
- Produce 1 online training course by month 12 of the project.
- Produce 3 on-demand short webinars aimed at managers in SMEs by month 18 of the project.
- Produce 6 blog posts that would be interesting to a variety of SME readers in the first year of the project.

We have discussed these targets throughout this document and most have been successful with two on-going: developing strategic partnerships and the SME training event. The one exception is the task to look at print and digital media, which we have since realised project funds cannot be used for.

6.2.2 Targets

We also set the following targets:

- Using a variety of internet-based sources, identify 280 new leads.
- Increase POP Twitter followers from 500 to 1000.
- Acquire 2 new SME users through our improved digital presence.
- Acquire 40 new SME leads from events by the end of the project.
- Attract 30 new SME leads through our engagement with professional bodies.
- Form one formal partnership with an HPC cloud provider by the end of the project.
- Acquire 5 new SME users through engagement with European organizations.
- Acquire 30 new SME leads from webinar registrations.

We set ourselves these above targets on lead generation to help us proportion the effort. Unfortunately, it is impossible to identify which business development activity brought in a particular user. Indeed, anecdotally, we believe people come to POP after engaging with several of our activities.

D4.1 reviews our social media presence including our twitter followers. Our twitter followers have been increasing and we should be able to meet the target, see D4.1 for more details.

As discussed earlier, a partnership with a cloud partner is still an on-going activity.

6.3 D2.2 Plan for Targeting CoEs

This deliverable presented the POP strategy for interacting with our fellow Horizon 2020 CoEs. We aimed to establish a communication channel to enable us to easily promote and provide POP services to them and collaborate on events and training.

6.3.1 Tasks

To strengthen the collaboration with other Horizon 2020 CoEs, we set ourselves the following tasks:

- Formally invite all CoEs to collaborate with POP.
- Establish a network with CoEs, with a single point of contact at POP.
- Identify which CoEs could benefit from POP services.
- Undertake Periodic Campaigns for all interested CoEs.
- Through our established network with CoEs, identify events where training or attendance would be beneficial.
- Through regular contact with CoEs, ensure that all possible collaborations are exploited.

As demonstrated in Section 3.1, we have accomplished all the above tasks. We are maintaining our relationships with other CoEs with ongoing conversations about organizing joint events, training workshops or further POP services where there is a need.

6.4 The Successes of POP So Far

With our milestones met, and our deliverable targets mainly so, POP business development is progressing well. Other notable achievements are the collaborations with HPC centres and online content. They are both new initiatives and could prove very successful and extremely cost effective.

Establishing collaborations are a very good way to embed the POP methodology into the HPC community and promote the POP brand. Once an external site is using the POP metrics and advertising our services, we would receive new users with virtually no effort.

Online content, once produced, has a long life. The videos will only need to be updated if there is significant change to the tools or metrics, although we have reduced the risk of needing to do this by making the videos quite short. If a new tool feature is added or a new POP metric devised, a new tutorial could be added to the list. It is also very easy to see how many people are using the resources and thus how effective they are being. Early indications are very positive.

7. Conclusion

Building on the previous POP project, we have extended our knowledge of the market. We have an ongoing strategy defined by our previous deliverables, the sectors we are targeting and our plans for the latter half of the project. We understand more fully the effort required to find a new user purely by marketing alone.

Many of our initiatives provide a mechanism for contacting a large number of potential users, including our work with professional bodies and external HPC

centres. This is not only cost effective but helps see how the business development activity could be sustainable.

Another initiative we believe will give real value for money is the generation of adaptable marketing material. It is not burdensome to create a flier for a new sector, for example, with just a little new text added to the established templates.

We have greatly expanded our digital content and done so in an adaptable way. We can add new online training modules, or record a new *POPCast*, to highlight advances in the project and are able to monitor the views made of them.

With three possible models identified we are on a path to deciding what the best approach is to make POP and its services sustainable.

8. Appendix

8.1 Events Attended for Business Development

Table 8: Events attended by POP for Business Development

Event Name	POP Partner(s) Attending	Activity	Location	Audience	Size of Audience (if known)
DOE Salishan HPC Konferenz	JSC	Talk "ROI of Performance Analysis of HPC Applications"	Salishan, US	Scientific, Academic & Industry	130
CCDSC 2018	JSC	Talk "ROI of Parallel Performance Optimization"	Lyon, FR	Scientific, Academic & Industry	60
RuSCDays 2018	JSC	Talk "On the ROI of Parallel Performance Optimization"	Moscow, Russia	Scientific, Academic & Industry	300
High Visual Computing 2019	IT4I	Talk	Czech Republic	Computer Graphics Community	40
RSE London	NAG	Talk	UK	RSE Community	
Workshop at Czestochowa University of Technology	IT4I	Talk	Poland	HPC and IT Community	14
9th JLESC Workshop	JSC	Talk "POP - The Quest for Performance Continues"	Knoxville, US	Scientific & Academic	120
Quant Minds	NAG	NAG Booth with POP fliers and digital content	Austria	Finance	
The EuroHPC Summit Week 2019	IT4I	Poster	Poland	HPC	
EuroHPC Summit Week 2019	Teratec	Attending	Poland	HPC Community	360

HPCSE 2019	IT4I	Talk & Poster	Czech Republic	HPC in CAE	96
Sickit Forum,	Teratec	Attending	France	Finance and Insurance Community	50
European Association of Geoscientists and Engineers	NAG	Attending	London, UK	Oil and Gas	
Annual Teratec Forum	Teratec	Workshops & Exhibition	France	HPC and IT Community	1300
Platform for Advanced Scientific Computing (PASC)	NAG	Talk & Poster	Switzerland	General HPC	
ISC HPC 2019	BSC, HLRS & JSC	Research exhibition booths	Germany	Academic & Industry	3500
PRACE Booth ISC HPC 2019	JSC	Booth Talk "POP - We are the "Performance" in HPC	Germany	Academic & Industry	30
Workshop at ICPP 2019	HLRS	Talk "MPI Collectives for Multi-core Clusters: Optimized Performance of Hybrid MPI+MPI Parallel Codes"	Japan	Academic	
Modelling 2019	IT4I	Plenary Talk	Czech Republic	HPC & IT Community	135
ScalPerf 2019	JSC	Talk "On the ROI of Parallel Performance Optimization"	Bertinoro, Italy	Scientific Academic & Industry	30
CompBioMed Conference 2019	NAG	Talk(s)	UK	Bio Community	
SPPEXA Final Symposium	JSC	Talk "Performance Tool Development for Exascale Systems"	Dresden, Germany	Scientific, Academic & Industry	120

International CAE Conference 2019	NAG	POP booth manned by NAG	Italy	CAE Community	
3rd SMEs workshop: Reducing Barriers to HPC Adoption for SMEs	HLRS	Talk	UK	Academic & Industry	25
SC19	BSC, HLRS, IT4I, JSC & NAG	Research exhibition booths	US	Academic & Industry	14
Advances in Computational Biology Conference 2019	BSC	Talk	Spain	Academic & Scientific	190
ORAP Forum	Teratec	Networking	France	Academic & Scientific	80
BioFIT	NAG	Booth w/ Focus CoE	France	Bio	
Austrian HPC Meeting 2020	IT4I	POP2 project poster and flash talk,	Austria	Academic; Industry	120
Energy Efficiency in HPC (PTC course) at IT4I	IT4I	Short talk about POP2 services: Energy Efficiency in HPC	Czech Republic	Academic	20
High Visual Computing 2020	IT4I	Poster, fliers	Czech Republic	Academic	90
Introduction to CFD Siegen	HLRS	Talk	Germany	CFD Community	15
10th NIC Symposium	JSC	Poster	Juelich, Germany	Academic	200

8.2 Professional Bodies Contacted

Table 9: Professional Bodies Contacted

Organisation Name	Website	Sector	Point of Contact
ANSYS	https://www.ansys.com/products/release-highlights	Pharma	NAG
Atlanpole	https://www.atlanpole.fr	Health	NAG
Clubster NSL	https://www.clubster-nsl.com	Health	NAG
Czechia.ai	https://www.aiczechia.cz	Artificial Intelligence, Czech Republic	IT4I
CzechInno	https://czechinno.cz/en/	Coordinator of all DIHs in Czech Republic	IT4I
DHUNE	https://dhune.org	Health	NAG
EFPIA	https://www.efpia.eu/manifesto/	Pharma	NAG
European Materials Modelling Consortium	https://emmc.info	Material Modelling	NAG
European Research Community on Flow, Turbulence and Combustion	https://www.ercoftac.org/	CFD	NAG
European Research Community on Flow, Turbulence and Combustion	https://www.ercoftac.org/	CFD	NAG
European Research Community on Flow, Turbulence and Combustion	https://www.ercoftac.org/	CFD	NAG
Innovate UK Knowledge Transfer Network	https://www.ktn-uk.co.uk/	Accelerator	NAG
JIC	https://www.jic.cz/en/	Business Support & Consultancy, South Moravia, Czech Republic	IT4I
Materials and Molecular Modelling	https://mmmhub.ac.uk/	Materials Modelling	NAG

MSIC	https://www.ms-ic.cz/en/	Moravian-Silesian Innovation Center, Czech Republic	IT4I
NAFEMS	https://www.nafems.org/	Engineering	NAG
Pistoia Alliance	https://www.pistoiaalliance.org/about/	Pharma	NAG
Prg.ai	https://prg.ai/en/	Artificial Intelligence, Czech Republic	IT4I
Syntec Numérique	https://syntec-numerique.fr/	Digital service companies, software Editors and technology consultancy companies	Teratec
Systematic Paris-Region Deep Tech Ecosystem	https://systematic-paris-region.org/	Accelerator and Networking	Teratec
Turku Business Region	https://www.turkubusinessregion.com	Accelerator and Networking	NAG
UK HPC SIG	https://hpc-sig.org.uk/	HPC	NAG
UK National Composites Centre	https://www.nccuk.com	Engineering	NAG
Vitagora	https://www.vitagora.com/en/	Food and Agri-business	Teratec

8.3 Marketing Materials

Examples of some of the marketing material produced for POP.

8.3.1 Pop-Up Banner



Figure 1: Pop-Up Banner Artwork

8.3.2 The POP Brochure

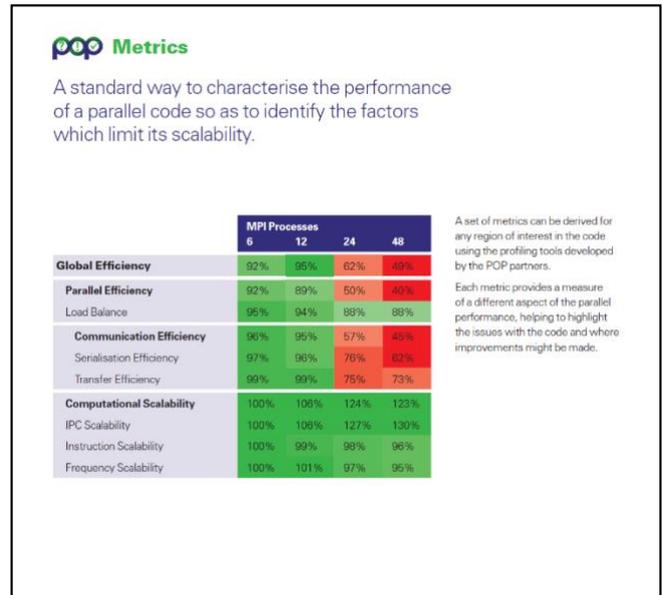
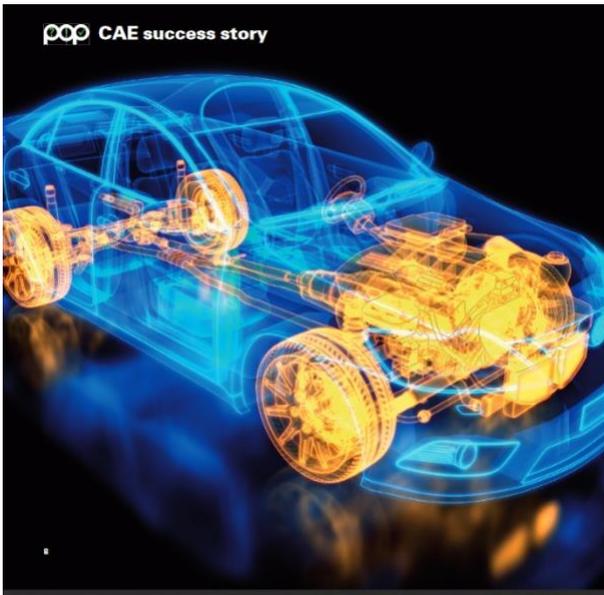
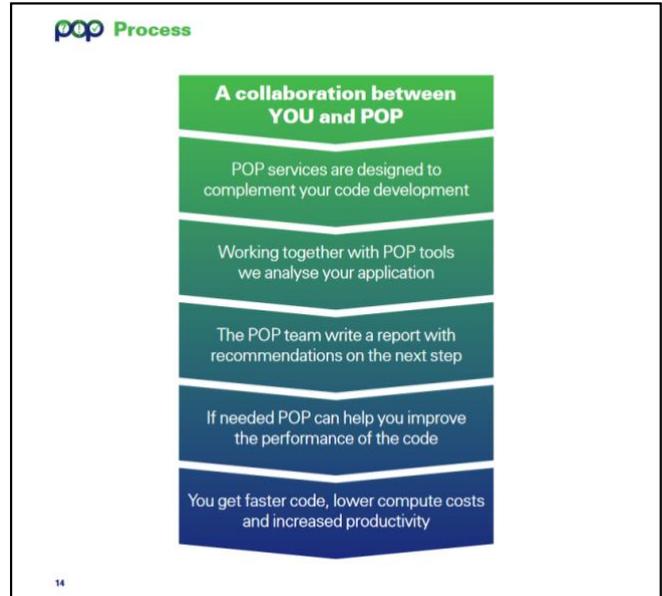
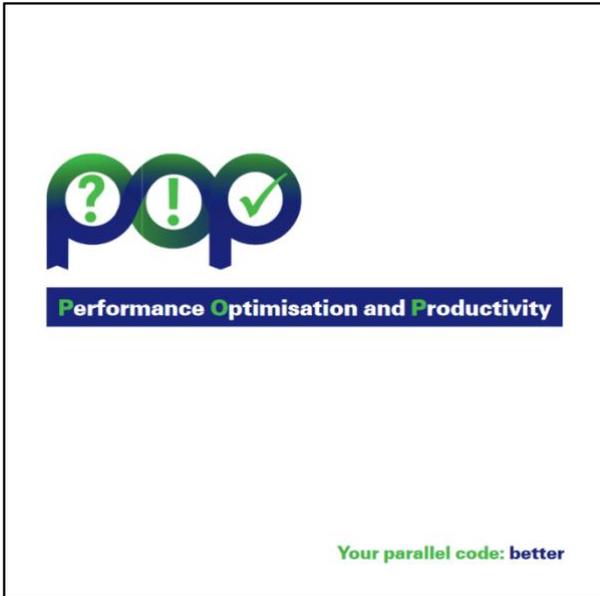


Figure 2: Example Pages from the POP Brochure

8.3.3 Sectoral Fliers



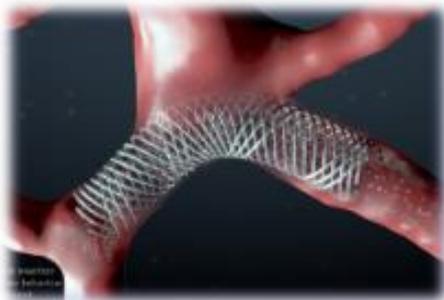
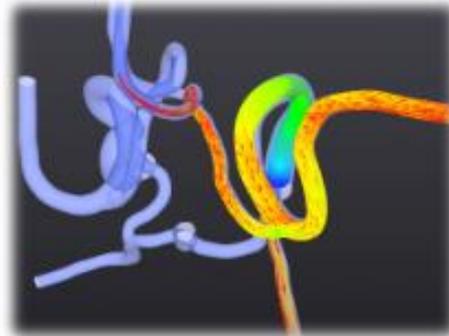
Performance Optimisation and Productivity



Performance Optimisation for Computational Biology

Collaboration between POP and CompBioMed to bring haemodynamics simulation to the exascale

Experts from FZ-Jülich worked with the CompBioMed CoE to optimise the flagship HemeLB (www.hemelb.org) blood flow simulation code.



POP provided expert analysis of HemeLB running on the Archer, Blue Waters and SuperMUC-NG HPCs, leading to some important optimisations:

- Memory requirements were reduced allowing larger simulations to be run.
- Improved load balance reduced time to solution, achieved through collaboration with E-CAM.
- Can now simulate over 10 billion lattice sites on the >300,000 core SuperMUC-NG (#9 Top500 HPC).
- Further collaborations with LRZ have developed higher performance visualisation solutions.

Your parallel code: better

Figure 3: Example of a POP Sectoral Flier (front) Computational Biology



A Centre of Excellence promoting best practice in parallel programming

- Providing FREE services giving a precise understanding of application performance and system behaviour
- Advice and support on how to refactor code in the most productive way
- Available for EU academic and industrial codes and users

HPC facilities are a major capital investment and often run close to capacity. Improving the efficiency of application software running on these facilities either speeds up time to solution or allows for larger, more challenging problems to be solved. The Performance Optimisation and Productivity (POP) Centre of Excellence exists to help you identify how your software can be improved, free of charge.

Funded by the EU under the Horizon 2020 Research and Innovation Programme, POP puts the world-class HPC expertise of eight commercial and academic partners at your disposal. POP has the tools and expertise to analyse all aspects of performance from single processor efficiency to the scalability of large parallel codes. We work with programs written in most languages and parallel paradigms, including MPI, OpenMP, CUDA, OpenCL and OpenACC.

Our analysis will identify issues such as memory bottlenecks, communication inefficiencies and load imbalances. This allows for a better understanding of

program efficiency and the identification of target kernels for code refactoring. We can work on these computational kernels and advise how to roll out improvements to your whole application. As well as reducing run-times, greater efficiency can also lead to reduced power consumption or cloud computing costs. In the first phase of POP we investigated thirty-four codes used by a range of commercial organisations and achieved an average performance improvement over the whole application of 2.25x, i.e. on average we more than halved the time to solution.

Our experience shows that it is often difficult to build a quantitative picture of HPC application behavior. One of the strengths of POP is our set of Metrics. They provide a standard, objective way to characterise different aspects of the performance of parallel codes. These simple measures, the performance data and recommendations are presented to you in a POP Performance Assessment report. This could be followed up by further work, again free to the user, to demonstrate the improvements that those recommendations would make.

Visit the POP Website for learning materials, our blog, and details of how to sign up for our newsletter and webinar programme.

www.pop-coe.eu

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[@POP_HPC](https://twitter.com/POP_HPC)



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

Figure 4: Reverse of all Sectoral Fliers



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Power consumption represents a significant cost factor in the overall HPC system economy. For these reasons researchers, supercomputing centers and major HPC vendors have developed new tools and methodologies to measure and optimize the energy consumption of large-scale high performance system installation.

POP offers to improve the energy efficiency of HPC applications using the methodology of dynamic tuning developed under the H2020 READEX project. This methodology has been designed for exploiting the dynamic behavior of parallel applications.

POP uses the MERIC tool developed at IT4Innovations that implements the READEX methodology and supports manual and binary instrumentation of the analyzed applications which is used to identify the significant regions in the HPC application.

MERIC first finds the optimal settings of hardware parameters (CPU core and uncore frequency, number of threads, ...) for all significant regions to create a so called tuning model.

Then for production runs MERIC performs the dynamic tuning of hardware parameters (applying

settings from the tuning model) as an HPC application progresses from one significant region to another.

This methodology has been thoroughly evaluated within the READEX project using both benchmarks as well as complex HPC applications. One can see that approximately 20% of energy savings is achieved across the various applications and we believe that similar savings can be achieved for new applications without any code modification.

Application	Hardware parameters	Savings Energy /time
AMG2013	CF, UCF, num. of threads	7.8% / -14%
Blasbench	CF, UCF, num. of threads	15.3% / -18.1%
Kripke	CF, UCF	18.8% / -18.7%
Lulesh	CF, UCF, num. of threads	18.7% / -11.7%
NPB	CF, UCF, num. of threads	10.8% / -12%
BEM4I	CF, UCF, num. of threads	34.1% / 10.9%
INDEED	CF, UCF, num. of threads	19.5% / 14.2%
ESPRESSO FEM	CF, UCF, num. of threads	33.0% / 22.2%
OpenFDAM	CF, UCF	20.1% / 11.5%

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Figure 6: Energy Saving Flier Reverse

Acronyms and Abbreviations

- BioExcel - The European Centre of Excellence for Biomolecular Research
- BSC – Barcelona Supercomputing Center
- CAE – Computer-Aided Engineering
- CFD – Computational Fluid Dynamics
- ChEESE – Centre of Excellence for Exascale in Solid Earth
- CoE – Centre of Excellence
- CompBioMed – Computational Biomedicine (CoE)
- D – Deliverable
- DIH – Digital Innovation Hub
- DoA – Description of Action (Annex 1 of the Grant Agreement)
- EC – European Commission
- E-CAM - The European Centre of Excellence for Software, Training and Consultancy in Simulation and Modelling
- EMMC – The European Materials Modelling Council
- EoCoE – The Energy-Oriented Centre of Excellence
- ESIWACE – The Centre of Excellence in Simulation of Weather and Climate in Europe
- EXCELLERAT - The European Center of Excellence for Engineering
- GA – General Assembly / Grant Agreement
- HiDALGO - HPC and Big Data Technologies for Global Systems (CoE)
- HLRS – High Performance Computing Centre (University of Stuttgart)
- HPC – High Performance Computing
- HPDA – High Performance Data Analytics
- ICHEC – Irish Centre for High-End Computing
- ISV – Independent Software Vendor
- IT4I – IT4Innovations (National Supercomputing Centre, VSB-Technical University of Ostrava)
- JSC – Juelich Supercomputing Centre
- KPI – Key Performance Indicator
- M – Month
- MaX – Materials Design at Exascale (CoE)
- NAFEMS – The International Association for the Engineering Modelling, Analysis and Simulation Community
- NAG – Numerical Algorithms Group
- PM – Person month / Project manager
- POP – Performance Optimisation and Productivity (CoE)
- PU – Public
- RSE – Research Software Engineering
- RWTH Aachen – Rheinisch-Westfaelische Technische Hochschule Aachen
- SMEs - Small and medium-sized enterprises
- UVSQ - Université de Versailles Saint-Quentin-en-Yvelines
- VI-HPS – Virtual Institute – High Productivity Supercomputing
- WP – Work Package

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i POP2 Deliverable D2.1 Plan for Targeting SMEs.

ii POP2 Deliverable D2.2 Plan for Targeting CoEs.

iii European Investment Bank Advisory Services, *Financing the future of supercomputing : How to increase investment in high performance computing in Europe:*

https://www.eib.org/attachments/pj/financing_the_future_of_supercomputing_en.pdf,
European Investment Bank, 201 p36

iv Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique.
<https://cerfacs.fr/en>

v Commissariat à l'énergie atomique et aux énergies alternatives. <http://www.cea.fr>

vi Centre national de la recherche scientifique. <http://www.cnrs.fr>

vii EMMC International Workshop 2021. <https://emmc.eu/events/emmc-international-workshop-2021/>

viii POP 2 Deliverable D4.1 First POP Dissemination and Training Report.

ix Partnership for Advanced Computing in Europe. <https://prace-ri.eu>

x POP Online Training. <https://pop-coe.eu/further-information/online-training>

xi POP blogs tagged as of interest to SMEs. <https://pop-coe.eu/blog/tags/sme>

xii BIOS IT, Information Technology & Services. <https://www.bios-it.co.uk/>

xiii Society of Research Software Engineering. <https://society-rse.org/>

xiv Digital Innovation Hub, Ostrava. <https://www.it4i.cz/dih-2/dih-info/?lang=en>

xv POP2 Deliverable D3.2 Customer Feedback Measurement.

xvi Virtual Institute - High Productivity Supercomputing. <https://www.vi-hps.org/>

xvii PyPOP. <https://github.com/numericalalgorithmsgroup/pypop>

xviii Cube. <https://www.scalasca.org/software/cube-4.x/>

xix BASIC ANALYSIS, download from: <https://tools.bsc.es/downloads>