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D7.5
Final Dissemination, Communication, Collaboration, Community Building and Standardization Report

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Author(s):	Sophia Honisch		USTUTT
	Antoine Dauptain		CERFACS
	Simon Loosen		RWTH
	Marie-Françoise Gerard Lucile Garnier		TERATEC
Approved by	Executive Centre Management		
Reviewer	Martina di Renzo		CINECA
Reviewer	Samir ben Chaabane		TERATEC
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List of abbreviations

AHM	*All Hands Meeting*
BoF	*Birds of a Feather*
CFD	*Computational Fluid Dynamics*
CoE	*Centre of Excellence*
CPU	*Central Processing Unit*
D	*Deliverable*
DLB	*Dynamic Load Balancing*
EU	*European Union*
ESS	*Exploitation Strategy Seminar*
F2F	*Face-to-face*
GPU	*Graphic Processing Unit*
HPC	*High-Performance Computing*
HRB	*Horizon Results Booster*
IG	*Interest Groups*
ISV	*Independent Software Vendor*
KER	*Key Exploitable Result*
KPIs	*Key Performance Indicators*
MPI	*Message Passing Interface*
SeRC	*Swedish e-Science Research Centre*
WP	*Work package*

Executive Summary

This document reports on the final activities of Work Package (WP7) until M42 with subsections for performed actions in the areas of dissemination, communication, collaboration, community building, and standardisation. These activities as a whole contributed to increasing EXCELLERAT's visibility as a Centre of Excellence for Engineering Applications, and raised the target audiences' awareness to be recognised as a partner for mutually beneficial collaborations and a vital part of the community. The final status of the KPIs reflected in this report indicates a strong performance of this work package.

After having built the EXCELLERAT brand and created an initial awareness about the project, WP7 disseminated and leveraged the results, outcomes and impact of the CoE's technical work. In addition to the established EXCELLERAT communication channels (website, Twitter, LinkedIn, blog, newsletter, press relations, podcast), WP7 supported the creation of white papers and scientific publications, produced 15 success stories and a total of nine promotional e-flyers, as well as two videos. In addition, in May 2022, WP7 successfully organised the virtual EXCELLERAT conference to highlight the overall achievements of the project.

Essential elements for the efficient integration of EXCELLERAT into the engineering HPC community are well-planned collaborative activities with European and national research projects, companies and dedicated research groups. To this end, new external partners were identified in the collaboration task such that the EXCELLERAT partners were able to establish new contacts and cooperation leading to a considerable collaboration network. In order to make the results of the collaboration, its accompanying unique value and services offered by EXCELLERAT visible to the engineering community, targeted success stories were established and disseminated via the EXCELLERAT website and social media channels.

Despite the additional challenge represented by the COVID-19 outbreak in March 2020, EXCELLERAT WP7 achieved to organise or attend several key events (e.g. NAFEMS World congress, a joint CoEs technical workshop or a Fortran webinar) in their online version to continue to interact with various audiences and to develop the community building of the project. To this end, WP7 created suitable communication material to be used for online promotion and for interaction with visitors of this new type of online events. Therefore, overall, EXCELLERAT successfully interacted with various communities of potential users or customers from the academic and industrial ecosystem throughout the whole project and the COVID-19 pandemic.

Although international standards may not strictly apply to EXCELLERAT's scope, standards from mainstream computing science were investigated and adapted by EXCELLERAT to the needs of the HPC community. Best practices on these investigations and a white paper were released.

As an outlook, this document further includes an outline of activities showing the sustainability of WP7 beyond the end of the project runtime.

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1 Introduction

The Centre of Excellence (CoE) for Engineering Applications EXCELLERAT aimed at boosting High-Performance Computing (HPC) for engineering to Exascale and thus enabling the engineering industry to use highly scalable codes leading to increased competitiveness. In order to help establish EXCELLERAT as a principal hub for industrial and academic players in the field of engineering with use of HPC, awareness about the services and expertise of EXCELLERAT was created among its stakeholders, which made it necessary to implement an effective communication and collaboration strategy.

The dissemination and communication strategy outlined in D7.2 [1] addressed the questions of how information was exchanged within the project, what communication goals and which target groups EXCELLERAT aimed to reach, as well as the message the project wanted to deliver to each of them. This is briefly summarised for the necessary context in section 2.1 of this document. In addition, communication and dissemination performance evaluation is outlined with the help of KPIs in section 2.2. This document explains the specific communication measures and tools the project used in order to meet the strategy outlined in the prior sub-section. The specific purpose of the EXCELLERAT portal is only briefly outlined, as it has been described in more detail in WP5 deliverables D5.4 [2], D5.5 [3], D5.6 [4], and D5.7 [5].

Additionally, in section 3, this deliverable provides a comprehensive summary of the activities, which were performed in cooperation with partners, projects, and other organisations beyond the EXCELLERAT Centre of Excellence, even to be maintained after the project runtime. Efficient collaboration on various levels was identified and continuously extended, e.g., with other European CoEs or projects, with industry companies and with national projects/partners working on HPC-related fields.

This document also reports on the activities contributing to community building (see section 4) as a tool to support the awareness creation of the EXCELLERAT project and brand and the promotion, and exploitation of the EXCELLERAT services more efficiently.

As outlined in section 5, the standardisation task published best practices on software versioning, data validation and production monitoring. A white paper detailed what and how production figures can be extracted from actual HPC production runs. Several open-source tools were released to ease the dissemination and enforcement of standards.

This document is the final report about WP7; it is the update of the initial version from M12 (see D7.3 [6]) and the updated report from M24 (see D7.4 [7]). It includes all activities until M42 of the project and gives an outlook on the sustainability of EXCELLERAT's WP7 activities.

2 Dissemination and Communication

The EXCELLERAT CoE's overall goal was to act as a single access point to technology and expertise for HPC applications in the engineering sector. Using the knowledge pool of EXCELLERAT should provide benefits to academia and industry. This easy and centralised access gives all parties the chance to free up their own resources to thrive on niche innovations specific to a particular code.

2.1 Goals and tools of dissemination

EXCELLERAT's outreach strategy combined both dissemination and communication. The activities of WP7 during the first half of the project focused more strongly on communication measures that aimed at building the EXCELLERAT brand and mainly awareness creation. Communication activities included the design of the logo and brand, the setup of the project's communication channels (website, blog, newsletter, social media accounts, podcast, media relations), identifying the optimal way of building a strong community, initiating standardisation tasks and creating a collaboration roadmap.

In terms of dissemination, WP7 focused on tailoring the outcomes and impact of the technical work to the target audiences' needs, distributing them accordingly, and thus exploiting them. Activities of dissemination included the creation of white papers and scientific publications, the development of success stories and e-flyers, the production of two EXCELLERAT videos, and the organisation of a virtual EXCELLERAT conference. The goals of the dissemination and communication strategy were achieved according to the reached KPIs at M42, as well as reflected in numerous success stories and in further outputs (see sections 2.2.3 and 2.2.4 for more details).

2.2 Progress with dissemination KPIs

Table 1 below shows the current values of the communication KPIs until M42 (May 2022) of the project. The goal was, amongst other things, to increase the traffic on our website and service portal in a way that it is not about numbers, but that the visitors get aware of the added value of EXCELLERAT and thus enter in discussions with the consortium. While the focus in the first half of the project was more on communicating about the project and building the EXCELLERAT brand and community, in the second half of the project WP7 put emphasis on the dissemination of the project's results, outcomes, collaborations, and impact (e.g. via success stories, scientific publications, white papers, and multimedia content).

Most of the KPI targets set could be achieved in M42 (see Table 1), with many of them, like the project presentations, LinkedIn followers, press clippings, newsletter subscribers, and website visitors, being overachieved. This is a proof of the good performance of EXCELLERAT's communication and dissemination activities. Some of the papers submitted to scientific publications are still under review, which is not unusual given the long review process of these famous scientific magazines. These publications are expected to be released in the next couple of months after the project end. The slightly lower number of total Twitter followers can be mitigated with the enormous outperformance of the EXCELLERAT LinkedIn account (reaching more than twice the number set in the initial targets). In discussion with the members of the Interest Groups, topics for a last workshop were identified. These were finally incorporated in the programme of the EXCELLERAT Online Conference in May 2022 for a wider reach. In addition to this, Interest Groups members were regularly informed about digital events and conferences with a presence of EXCELLERAT.

Tool	KPI	Status M42	Target M42
Publication	Released Scientific Papers and Conference Proceedings	39 (incl. 1 in press, 5 not yet released) + 2 to be submitted	35
	Press Releases	4 (incl. final one to be released after project end)	4
	Released White Papers	5	5
Events	Project presentations conferences/events	42 (+ 2 planned after project end)	25
	Significant presence at events (hosted, sponsorship and booths)	29 (incl. workshops and webinars) + 3 planned after project end)	15
	No. of Workshops/Interest Groups meetings | no. of workshop participants	3 | in average 14 participants per workshop/meeting	4 workshops Interest Groups meetings
	No. of conferences | No. of attendees	2 | 133	2 | Total 150
Social Media	No. of twitter postings, Followers, Engagement and Impressions	926 tweets 528 followers 1.39% average engagement rate in average 679 Impressions/tweet	Regular postings, 200 Follower p.a. & 500 impressions
	No. of LinkedIn postings, followers, engagement and impressions	309 postings 508 followers, 6% average engagement rate in average 2,807 impressions	75 Followers p.a., 300 impressions
Reference in external media channels (on- & offline)	Press clippings	34	20
EXCELLERAT Website	Number of visitors	Overall 138,293 (until 24/05/22)	7,000 p.a.
EXCELLERAT Portal	Number of subscribers	68 active users (51 internal, 17 external)	50
Newsletter	Number of subscribers	155	150

Table 1: KPIs Overview

2.2.1 Website

The EXCELLERAT website [8] architecture and analytics have been addressed in great detail in deliverable D7.1 "Website, Corporate Design and Templates" [9]. The most important statistics are the following:

- Overall unique visitors (sum of monthly visitors from M1-M42): 138,293
- Top referring Domains: Google, Twitter, ssc-services.de, LinkedIn, baidu.com, bit.ly, hpccoe.eu.
- Search terms: excellerat european center, success of high performance computing, excellerat, excellerate eu project, ecerfacs combustion.
- Top visited pages: Home, Blog, Expertise, Our Goals, Newsletter, Success Stories, Partners, News, Services

As reported in D7.4 [7], the website was re-designed and restructured in June 2020 for a better user experience. The website was continuously updated with new content and minor style edits. The website performance statistics and evolution of unique visitors prove the success of this redesign and content strategy, since the number of unique visitors has significantly increased after June 2020 (see Figure 1). In addition, with major support of WP7, WP5 adapted the design of the service portal to the redesigned website in early 2021. The service portal is now better incorporated into the project website, with cross-links and several subpages embedding the service portal directly (e.g. services, training and events), and a call to action to visit the service portal on the homepage of excellerat.eu. This is further outlined in D5.7 [5].

The domain www.excellerat.eu will remain online at least until 2023. In case of a second funding phase of EXCELLERAT, the same website domain of the first project phase could further be used without any issues.

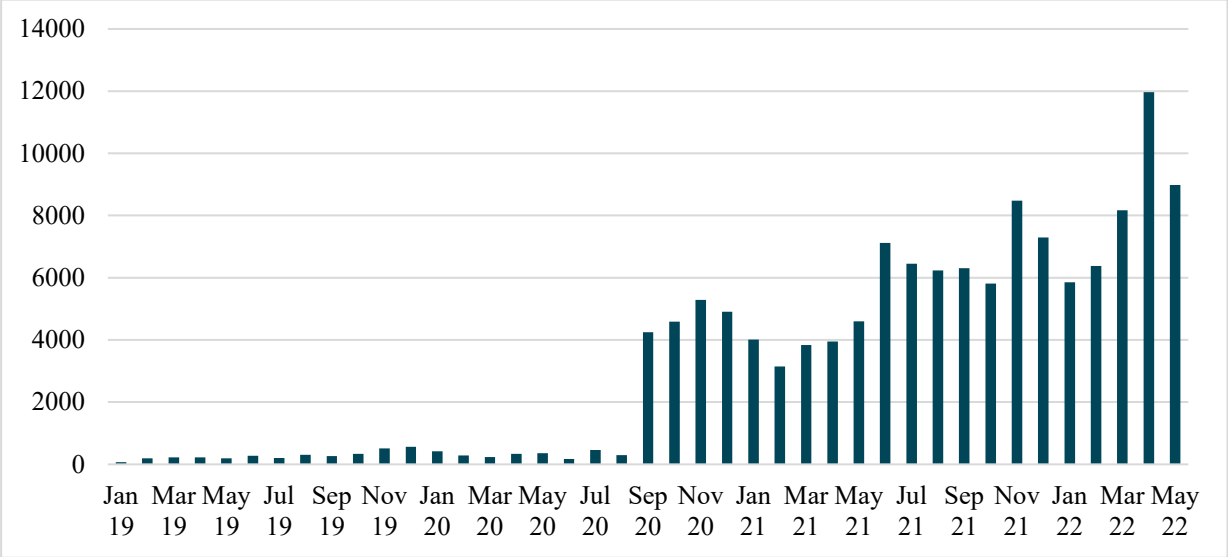

Figure 1: Monthly unique website visitors excellerat.eu

2.2.2 Newsletter, Publications and White papers

The bi-monthly EXCELLERAT newsletter [10] was set up with the first issue being released in May 2020. The first issue was published in .pdf format, since the updated website was not yet released at that time. From issues two until 12 (last one released in April 2022) were integrated into the website and regularly sent out via the WordPress plug-in MailPoet [11] which had previously been used by FocusCoE and other Centres of Excellence, like BioExcel and MaX CoE. This plug-in had several advantages, e.g. it increased the visibility via Google search, it was more accessible via smartphone than a PDF, it was easy to maintain and manage the subscribers and mailings in one single place, and, together with the according data policy form, it complied with the GDPR regulation. In month 42 (M42), 12 issues have been released. The newsletter will be maintained on a regular basis beyond the project end. 155 persons have subscribed to the newsletter mailing list. This mailing list will be kept beyond the project end so that in case of a second funding phase the consortium can build on an existing readership for re-initiated newsletter activities, with the aim to further extend this community.

The newsletter generally consists of various sections: an introduction by the Project Coordinator, a success stories section, a part that highlights one of EXCELLERAT's blog articles, as well as events and further news sections, which include e.g. new podcast episodes, website updates or related news. The newsletter was sent out bi-monthly via e-mail to the list of subscribers, it was regularly promoted via Twitter and LinkedIn, and the archive will remain embedded on the website in the newsletter section [10].

32 scientific papers (see Annex 1) were published in research journals and conference proceedings, such as IEEE conference proceedings. This number has constantly increased with more scientific results, with many conferences postponed to 2021 due to the COVID-19 pandemic. One paper is still in press, five papers have not yet been released due to long review phases and are expected to be published a few months after the project end. Two publications (one in a journal, one conference proceeding) will be submitted after the project end.

As described in D7.4 [7] WP7 developed a white paper concept with a respective structure template and a specific definition of white papers and their purpose for EXCELLERAT.

The definition and concept of white papers include:

- A technical, objectively/unbiased written document that elaborates innovations developed in EXCELLERAT with convincing (but not sales kind of) arguments, statistics/research results.
- Written for an expert audience, like (research) software developers, ISVs, etc.
- The intro and outro are very important, as they are most likely to be remembered by the readers – this should catch the interest. The text shall be more detailed than a blog article but still interesting. Success stories can be a helpful basis for the storyline of a white paper.
- This document should have between five and ten pages and it shall be written in an understandable language.
- Reference links can be included, tags and key words are useful for further categorisation.
- The white paper process shall include a review by a few EXCELLERAT members.

Purpose of white papers for EXCELLERAT:

- To promote a certain product/service/technology/methodology in a convincing way without an obvious marketing strategy, by factually presenting their benefits for potential stakeholders
- To influence decision making
- To generate leads
- Thought leadership
- To disseminate research results

The first white paper was created by the standardisation task in WP7 (see section 5) and released via the website [12]. This was helpful for testing and thus further improving the process and template. Four additional white papers were developed by WP1, WP3, and WP4 about the topics of uncertainty quantification and the tool UQit, the EXCELLERAT Data Workflow Platform, FPGAs for accelerating HPC engineering workloads: the why and the how, and based on the best practice guide. The white papers are available online [13].

2.2.3 Success Stories and e-flyers

As outlined in detail in D7.4 [7], a concept for **success stories** with different types of success stories was developed and implemented in order to reach all EXCELLERAT target audiences. In total, 15 EXCELLERAT success stories were released over the course of the project, with an increase towards the end of the runtime. The list of success stories is available in Table 2 below.

Title of Success Story	URL
Full Airplane Simulations on Heterogeneous Architectures	https://www.excellerat.eu/success-story-full-airplane-simulations-on-heterogeneous-architectures/
Enabling parallel mesh adaptation with Treeadapt	https://www.excellerat.eu/success-story-enabling-parallel-mesh-adaptation-with-treeadapt/
Towards an increased accuracy in the automotive field simulations	https://www.excellerat.eu/success-story-towards-an-increased-accuracy-in-the-automotive-field-simulations/
Bringing industrial end-users to Exascale computing: An industrial level combustion design tool on 128K cores	https://www.excellerat.eu/success-story-bringing-industrial-end-users-to-exascale-computing/
Enabling High Performance Computing for Industry through a Data Exchange & Workflow Portal	https://www.excellerat.eu/success-story-enabling-high-performance-computing-for-industry-through-a-data-exchange-workflow-portal/
Accelerating engineering codes using reconfigurable architectures	https://www.excellerat.eu/success-story-accelerating-engineering-codes-using-reconfigurable-architectures
Enabling Nek5000 on GPU systems	https://www.excellerat.eu/success-story-enabling-nek5000-on-gpu-systems/

Improving the HiDALGO CoE's Urban Air Pollution Pilot	https://www.excellerat.eu/success-story-improving-the-hidalgo-coes-urban-air-pollution-pilot/
A POP proof-of-concept allows a Bunsen flame use case from EXCELLERAT to run two times faster	https://www.excellerat.eu/success-story-a-pop-proof-of-concept-allows-a-bunsen-flame-use-case-from-excellerat-to-run-two-times-faster/
Enabling sustainable GPU acceleration on a Fortran legacy code	https://www.excellerat.eu/success-story-enabling-sustainable-gpu-acceleration-on-a-fortran-legacy-code/
A novel framework for online estimation of the uncertainties in turbulent flow statistics	https://www.excellerat.eu/success-story-a-novel-framework-for-online-estimation-of-the-uncertainties-in-turbulent-flow-statistics/
Accelerating Alya engineering simulations by using FPGAs	https://www.excellerat.eu/success-stories-accelerating-alya-engineering-simulations-by-using-fpgas/
Transparent Integration of Emerging HPC Technologies into the Computational Fluid Dynamics Software CODA	https://www.excellerat.eu/success-story-transparent-integration-of-emerging-hpc-technologies-into-the-computational-fluid-dynamics-software-coda/
Running AVBP Industrial code on Arm architectures	https://www.excellerat.eu/success-story-running-avbp-industrial-code-on-arm-architectures/
In situ VR visualisation of Nek5000 simulations with Vistle	https://www.excellerat.eu/success-story-in-situ-vr-visualisation-of-nek5000-simulations-with-vistle/

Table 2: List of EXCELLERAT success stories

As previously defined, the EXCELLERAT website served as a content hub for all success stories [14] and they will remain online beyond the project's end. Together with EXCELLERAT partners, the former WP7 team will continue to work on additional success stories after the project end, in cases where the results were not fully available by early May 2022. The success stories were further distributed via the newsletter, LinkedIn and Twitter, conference presentations and in e-flyers promoting the (potential) services of the CoE. These distribution channels were chosen for a maximum reach and engagement with several target audiences.

Based on discussions about the further promotion of the EXCELLERAT services and the service portal, WP7 conceptualised, coordinated, edited, and created a total of **nine e-flyers,** with the aim of showing the EXCELLERAT services, successes and benefits at a quick glance, especially to a busy target audience with limited time:

- Five flyers were created and classified by **focused topic of expertise**, showing the services and tools that EXCELLERAT can offer in these fields, which challenges they can solve, and their unique values and benefits in: data-management, simulation, visualisation, data analytics, co-design. An example can be found in Figure 2.
- Four flyers were created by EXCELLERAT's **industrial sector**, showing compact success stories that are relevant for each given sector: Aerospace, Energy, Automotive, Manufacturing. A visual example can be found in Figure 3.

The great advantage of creating targeted flyers with adapted frame (and consequent distinction by sector and topic) is that target audiences can be addressed with tailor-made content, even though some elements were included across several flyers (sectorial flyers). For instance, the aeronautics flyer is mainly directed towards industrial design engineers and experts from the aeronautics industrial sector, while the automotive flyer addresses R&D experts from the automotive industry, industrial R&D engineers, CFD users, code developers, and hardware providers.

The first set of flyers (five topic flyers and aerospace flyer) was initially launched as a follow-up communication to visitors of the NAFEMS World Congress booth in October 2021. They were updated at a later stage and completed with further sectorial flyers covering additional success stories when they were released. The flyers were and will still be provided in the downloads section of the EXCELLERAT website [15], they were shared via the newsletter and further distributed via direct mailing and the EXCELLERAT social media channels. In May 2022, the topic and selected sectorial flyers were produced as print material to accompany partners who visited the ISC High-Performance Conference in Hamburg, Germany. The initially created materials, as e-flyers, were adjusted to be suitable for print, e.g. with QR codes leading to the respective services and success stories. This aimed at further disseminating the achievements of EXCELLERAT and maintaining relevance even beyond the project end.

To boost EXCELLERAT's final performance, its services, the service portal, and the number of downloads of the flyers, four short animation videos (per sector) were further created in May 2022. Their purpose was to be used for paid promotions via LinkedIn. At the time of the writing of this report, these videos are being finalised.

Figure 2: EXCELLERAT Data Analytics Flyer

Figure 3: Cover of the EXCELLERAT Aerospace Flyer

In addition, as part of the dissemination of successful results of the project, a flyer showing selected innovations spotted by the EU Innovation Radar was created in June 2021 [16]. The general EXCELLERAT project's flyer created at the beginning of the project was also updated in January 2022 with a modernised design [17].

Figure 4: Extract of EXCELLERAT Innovations Flyer

2.2.4 Podcast, blog, and videos

As EXCELLERAT continued to follow a multi-media approach to communication, some of the blog articles and themes were enhanced by videos, podcasts, and flyers. Used formats include the following:

- **Podcast**: An HPC Podcast powered by EXCELLERAT has been developed, with a total of four episodes published. Episode #1 [18] was recorded with Sicos and dealt with an overall explanation of HPC; episode #2 [19] was released in collaboration with Pipistrel, a Slovenian SME for lightweight aircrafts, and focused on the main challenges faced in their product development; episode #3 [20] was an interview with ANSYS, the global leader in engineering simulation and a newer member of the EXCELLERAT Interest Groups. Finally, the episode #4 [21] was produced with Prof. Dr. Sabine Roller from the consortium partner DLR and dealt with the issue of how simulations could be applied to make aircrafts more environmentally friendly.
- **Blog**: A total of 38 comprehensive blog articles about recent development topics, events, and other news of the project were released via the blog subpage on the EXCELLERAT website [22]. A full list of the blog articles with release dates and URLs can be found in Table 3. The blog will be regularly updated beyond the project end.
- **Service animation video**: In coordination with WP5, WP7 produced an animation video with an expert from Arctur in order to promote the EXCELLERAT services and in particular the service portal. A storyboard and script were developed, visual material

was provided by EXCELLERAT partners and completed with suitable stock footage. The animated video was finalised and released in May 2021, hosted on the EXCELLERAT website [23] and distributed multiple times via the social media channels as well as the newsletter issue #7 [24].

- **Explanatory video**: Together with experts from the visualisation department of BSC, WP7 and WP1 produced an animated video [25] explaining the aim and achievements of the EXCELLERAT project to every target group visiting the website. A detailed storyboard, structure, and script were created based on simulations run by the EXCELLERAT partners. In the post-production phase, sound effects, voice-over, and subtitles were added. Once finalised and approved for launch at the NAFEMS World Congress [26] booth in October 2021, the video was published via BSC's YouTube channel and embedded at the bottom of the website's homepage, where it will remain. Until now, it has achieved about 600 views over YouTube and resulted in many social media likes interactions compared to other posts on EXCELLERAT's channels.

Date	Title of article	URL
February 17, 2017	New supercomputing record set by ANSYS, HLRS and Cray	https://www.excellerat.eu/new-supercomputing-record-set-by-ansys-hlrs-and-cray/
February 23, 2017	Scania cooperates with PDC to further improve its vehicles	https://www.excellerat.eu/scania-cooperates-with-pdc-to-further-improve-its-vehicles/
May 9, 2017	CERFACS and CNRS perform first-ever Large Eddy Simulation of combustion instabilities in a rocket engine	https://www.excellerat.eu/cerfacs-and-cnrs-perform-first-ever-large-eddy-simulation-of-combustion-instabilities-in-a-rocket-engine/
May 10, 2017	A French SME boosts its offshore engineering service portfolio thanks to European HPC initiatives	https://www.excellerat.eu/a-french-sme-boosts-its-offshore-engineering-service-portfolio-thanks-to-european-hpc-initiatives/
June 19, 2017	BSC and NVIDIA a step forward to the interactive simulation of humans	https://www.excellerat.eu/bsc-and-nvidia-a-step-forward-to-the-interactive-simulation-of-humans/
March 2, 2018	HPC helps to make combustion plants safe and cost-efficient	https://www.excellerat.eu/hpc-helps-to-make-combustion-plants-safe-and-cost-efficient/
May 3, 2018	EU-Project helps Engineering SME Improve Competitive Position	https://www.excellerat.eu/eu-project-helps-engineering-sme-improve-competitive-position/

December 21, 2018	EXCELLERAT to Bring HPC Applications to Engineering Industry	https://www.excellerat.eu/excellerat-to-bring-hpc-applications-to-engineering-industry/
February 12, 2019	New analysis methods facilitate the evaluation of complex engineering data	https://www.excellerat.eu/new-analysis-methods-facilitate-the-evaluation-of-complex-engineering-data/
June 4, 2019	Preparing Cloud Physics for Exascale	https://www.excellerat.eu/preparing-cloud-physics-for-exascale/
July 12, 2019	Importance of Data Transfer in the Use of High Performance Computing	https://www.excellerat.eu/importance-of-data-transfer-in-the-use-of-high-performance-computing/
July 31, 2019	Enabling the future of CFD for external aerodynamics optimization with exascale systems	https://www.excellerat.eu/enabling-the-future-of-cfd-for-external-aerodynamics-optimization-with-exascale-systems-2/
July 31, 2019	Enabling the future of CFD for safety applications with Exascale systems	https://www.excellerat.eu/enabling-the-future-of-cfd-for-safety-applications-with-exascale-systems/
August 29, 2019	Toward Quantifying Uncertainties in Large-Scale Simulations of Engineering Flows	https://www.excellerat.eu/toward-quantifying-uncertainties-in-large-scale-simulations-of-engineering-flows/
December 13, 2019	EXCELLERAT Team Meeting in Bologna (Nov 2019)	https://www.excellerat.eu/excellerat-team-meeting-in-bologna/
February 5, 2020	The Industrial HPC-User Roundtable focused on the computational challenges industry faces, with a special focus on the growing interest in solutions involving artificial intelligence.	https://www.excellerat.eu/the-ihurt-focused-on-the-computational-challenges-industry-faces-with-a-special-focus-on-the-growing-interest-in-solutions-involving-artificial-intelligence/
May 11, 2020	First virtual EXCELLERAT All Hands Meeting (May 2020)	https://www.excellerat.eu/first-virtual-excellerat-all-hands-meeting-may/
May 15, 2020	EPCC develops new modelling techniques for the chemical and oil and gas industry	https://www.excellerat.eu/epcc-develops-new-modelling-techniques-for-the-chemical-and-oil-and-gas-industry/
May 27, 2020	Dynamic Load balancing for Airplane simulations on	https://www.excellerat.eu/dynamic-load-balancing-for-airplane-simulations-on-heterogeneous-pre-exascale-architectures/

	Heterogeneous pre-Exascale architectures	
July 20, 2020	New EXCELLERAT Service Portal is launched	https://www.excellerat.eu/new-excellerat-service-portal-is-launched/
July 29, 2020	Nek5000 in EXCELLERAT: towards Exascale	https://www.excellerat.eu/nek5000-in-excellerat-towards-exascale/
September 4, 2020	EXCELLERAT collaborates with the HiDALGO Centre of Excellence	https://www.excellerat.eu/excellerat-collaborates-with-the-hidalgo-centre-of-excellence/
October 8, 2020	High-performance computing challenge: How can engineers effectively leverage HPC technology?	https://www.excellerat.eu/high-performance-computing-challenge-how-can-engineers-effectively-leverage-hpc-technology/
December 15, 2020	EXCELLERAT's Second Virtual All-Hands Meeting	https://www.excellerat.eu/excellerats-second-virtual-all-hands-meeting/
December 15, 2020	EXCELLERAT goes digital: 36th International CAE Conference and Exhibition	https://www.excellerat.eu/excellerat-goes-digital-36th-international-cae-conference-and-exhibition/
January 5, 2021	Gauging High Performance Computing needs for industrial applications: a worked example	https://www.excellerat.eu/gauging-high-performance-computing-needs-for-industrial-applications-a-worked-example-2/
February 10, 2021	EXCELLERAT's First Joint Technical Workshop with ChEESE and HiDALGO Centres of Excellence	https://www.excellerat.eu/excellerats-first-joint-technical-workshop-with-cheese-and-hidalgo-centres-of-excellence/
March 12, 2021	The use of in-situ analysis tools by EXCELLERAT	https://www.excellerat.eu/the-use-of-in-situ-analysis-tools-by-excellerat/
April 8, 2021	EXCELLERAT Training Workshop: Using Machine Learning To Analyse Engineering Data	https://www.excellerat.eu/excellerat-training-workshop-using-machine-learning-to-analyse-engineering-data/
June 11, 2021	EXCELLERAT's Third Virtual All-Hands Meeting	https://www.excellerat.eu/third-virtual-all-hands-meeting/
August 30, 2021	Road and Scouts: a versioning strategy for large Research software	https://www.excellerat.eu/road-and-scouts-a-versioning-strategy-for-large-research-software/

October 27, 2021	How can SMEs benefit from using High Performance Computing (HPC) Cloud	https://www.excellerat.eu/how-can-smes-benefit-from-using-high-performance-computing-hpc-cloud/
November 26, 2021	EXCELLERAT Exploitation Strategy Seminar with Horizon Results Booster for Vistle, Alya and Uqit	https://www.excellerat.eu/excellerat-exploitation-strategy-seminar-with-horizon-results-booster-for-vistle-alya-and-uqit/
December 6, 2021	EXCELLERAT's Fourth All-Hands Meeting	https://www.excellerat.eu/excellerats-fourth-all-hands-meeting/
January 19, 2022	Key points and take-outs from the FORTRAN webinar organised by EXCELLERAT	https://www.excellerat.eu/key-points-and-take-outs-from-the-fortran-webinar-organised-by-excellerat/
March 16, 2022	On the technical debt of high-performance scientific software	https://www.excellerat.eu/on-the-technical-debt-of-high-performance-scientific-software/
April 26, 2022	Data management workflow for HPC – SSC Data Management Workflow Portal	https://www.excellerat.eu/data-management-workflow-for-hpc-ssc-data-management-workflow-portal/
May 25, 2022	EXCELLERAT Conference: Impressions, Takeaways, and How to Watch	https://www.excellerat.eu/excellerat-conference-impressions-takeaways-and-how-to-watch

Table 3: List of EXCELLERAT blog articles

2.2.5 Social Media

EXCELLERAT used social media for promoting content and connecting with, as well as building its own community. In particular for EXCELLERAT, social media was exploited to:

- increase traffic to the website, a proof of this was that LinkedIn and Twitter are among the top referral pages
- create and engage a community interested in HPC engineering and Exascale technology
- promote the enlargement of the EXCELLERAT community, by achieving new subscribers to the EXCELLERAT Portal and newsletter and by reaching new users of EXCELLERAT services
- inform about upcoming events, news, newsletter issues, blog articles, new podcast episodes, success stories, multimedia content, and results from the project
- support the members, create another platform to interact and discuss topics directly
- engage and interact with the community with creative content, such as an HPC trivia quiz or #SimulationFriday, which also increases the engagement rate and probability of retweets

On Twitter and LinkedIn, WP7 continuously created and published content on behalf of EXCELLERAT, tagging the relevant partners' handles in posts in order to encourage engagement and to connect every partner with the community. As a measure of further boosting the performance of EXCELLERAT's social media presence, WP7 established a social media ambassador programme in March 2021. All partners were asked to provide a communication and social media representative from their institution, ideally with appropriate access to their social media channels. Some of these ambassadors also manage other EU-funded projects' social media accounts and thus are well-connected. This certainly helps to leverage the performance of EXCELLERAT's channels. A mailing list was set up with these ambassadors. WP7 developed a list of LinkedIn groups per relevant industrial sector for EXCELLERAT and asked the ambassadors to interact in these groups as much as possible. More than 70 contributions to these LinkedIn groups were reported to the WP7 leader by the ambassadors. In addition to the call for engagement with the LinkedIn groups and interaction with the EXCELLERAT social media channels, the ambassadors received weekly updates (in advance) of scheduled tweets and LinkedIn posts as well as highlights for the upcoming week. In this way, they were ready to give EXCELLERAT's posts additional reach and engagement across their institutions' channels and beyond. The engagement and number of likes increased notably since adopting this methodology.

Moreover, the social media banners were updated in the beginning of 2021 for a more modern look. Sharing news and scientific results, for example through success stories, and participating in events were highly important. Proximity to the community and interaction via social media, the website or personal contacts were key factors in the successful dissemination of EXCELLERAT's results and achievements. The social media channels will be maintained on a minimum level until at least 2023. In this way, pending publications and potential further news from the consortium can still be communicated to the EXCELLERAT community. Finally, this will facilitate the implementation of communication in a possible second phase of the project, in which the team could build upon an already existing community of followers.

2.2.6 EXCELLERAT Conference

The EXCELLERAT Online Conference [27] was mainly conceptualised and organised by WP7 with support from all other work packages and partners. The conference with the official title "EXCELLERAT: Enabling Exascale potentials for engineering applications" took place on 16 and 17 May 2022 via the online meeting tool WebEx and was open to a large audience, being organised through the event management platform Eventbrite.

The conference was dedicated to showcasing the impact, innovations and tools resulting from the project. This was targeted towards a large audience of stakeholders (academics, HPC hardware providers, code developers (ISVs), HPC cloud computing, AI providers) as well as (potential) customers (industrial end users, academics) with the objectives to extend the EXCELLERAT community, leverage the potential for future collaboration, showcase the relevance of EXCELLERAT to a broader audience, and to increase the number of potential users of the services. WP7 set the following KPIs to measure the success of the event:

- Get at least 2 VIP speakers for the event → This was achieved with a total of four guest speakers from industry, European Commission, and the EuroHPC Joint Undertaking, see agenda in Table 4 and Table 5.
- Achieve a minimum number of 60 participants, with at least 15% non-academic participants, from different target audiences and several European countries →

  - This was partly achieved. 73 people registered via Eventbrite and 15 additional persons from the EXCELLERAT consortium accepted the invitation via e-mail/calendar.
  - 15-17% of the registered persons were from non-academic organisations.
  - People from several European countries registered: Germany, France, Italy, Spain, UK, Slovenia, Hungary, Luxembourg, Sweden, Latvia, (Turkey), Switzerland, Ireland, Croatia, and beyond (e.g. USA).
  - On Day 1, the number of participants ranged from 47 to 60 (i.e. 53,5 average) participants. The majority was available before the break and a couple of participants were lost after the coffee break.
  - On Day 2, the attendance varied from 31 to 55 (i.e. 43 average) persons. This number was higher in between and at lower numbers after the break and in the end. Given this difference, the average for both days was at 48,25 participants.
- Get at least 10 mentions on social media from participants'/partners' channels:
  - 24 mentions of EXCELLERAT/shares on LinkedIn related to the conference
  - 36 retweets/mentions on Twitter related to the conference
- Achieve at least 10 newsletter and service portal subscriptions → 25 new newsletter subscribers, 2 new portal subscribers

In order to achieve these KPIs, WP7 developed a communication plan for wide promotion of the event in advance and for communications during and after the conference. This plan included the creation of a communication kit (see Annex 2) with standardised messaging (e-mail draft, website template text, newsletter and social media post suggestions) as well as visual content (see example in Figure 5) to be used for announcements. This communication kit was provided to the consortium partners (in particular to the social media ambassadors) and widely used for the promotion and distribution among their own networks. The promotion on behalf of EXCELLERAT was undertaken via Twitter and LinkedIn, as well as newsletter issue #12 [28], and direct mailing (Interest Groups, personal contacts). Individual talks were promoted via Twitter and LinkedIn shortly before the event took place.

Moreover, to push the registration rate towards the end, a LinkedIn paid promotion was placed from 11 to 16 May in the morning. This ad led to 77 clicks on the event page, 37,782 impressions in total, €5.79 average Cost per Click (CPC), and a total spent of €446.11. Registrations increased in the last few days from a total of 44 on 11 May (before the paid promotion was in place) to 73 by 16 May, when the ad and registration had closed.

In addition to this, event announcements were shared with the broader network of EU-funded projects, such as the European Centres of Excellence via the FocusCoE Slack channel, the European National Competence Centres via the EuroCC/CASTIEL Slack channel and the weekly EuroCC-internal newsletter, and social media shares.

Figure 5: Visual for Promotion of EXCELLERAT Conference

The programme consisted of an introductory talk from a representative of the European Commission, a speaker from the EuroHPC Joint Undertaking, and keynotes from two experts from the industry as special guests, as well as several talks from representatives of the EXCELLERAT consortium, presenting the highlights of the project's technical work. More details can be found in the agenda in Table 4 and Table 5.

Time (CEST)	Duration	Title	Speaker, Organisation
14:00-14:15	15 min.	Introduction: The EXCELLERAT Centre of Excellence	Ralf Schneider, HLRS
14:15-14:30	15 min.	HPC strategic priorities of the European Commission	Agne Cerniauskaite, European Commission
14:30-14:50	20 min.	The Journey of In-situ Visualisation with Vistle	Dennis Grieger, HLRS
14:50-15:05	15 min.	UQit: A Tool for Uncertainty Quantification in Fluid Engineering	Saleh Rezaeiravesh, KTH
15:05-15:15	10 min.	Q&A	Dennis Grieger, Saleh Rezaeiravesh
15:15-15:30	15 min.	Coffee break	-
15:30-16:00	30 min.	HPC and Cloud Computing Continuum for Aerospace Applications	Carlo Cavazzoni, Head of the Leonardo Labs Future
16:00-16:30	30 min.	Potential Exascale Applications of EXCELLERAT	Mark Sawyer, EPCC
16:30-16:35	5 min.	Closing of Day 1	Ralf Schneider, HLRS

Table 4: Agenda of Conference Day 1, 16th May 2022

Time (CEST)	Duration	Title	Speaker, Organisation
09:00-09:05	5 min.	Short introduction	Ralf Schneider, HLRS
09:05-09:35	30 min.	The Role of Industrialisation in the Adoption of HPC Code in the Industry	Julien Tillou, Head of Combustion Design Department, Safran Aircraft
09:35-09:50	15 min.	Computational Strategies for Efficient CFD Simulations using Dynamic Load Balancing	Guillaume Houzeaux, BSC
09:50-10:15	25 min.	GPU Acceleration Towards Exascale	Gabriel Staffelbach, CERFACS Michael Wagner, DLR Daniel Mira, BSC Adam Peplinski, KTH
10:15-10:25	10 min.	Coffee break	-
10:25-10:40	15 min.	Adaptive Mesh Refinement: A Summary of EXCELLERAT's Achievements	Gavin J. Pringle, EPCC
10:40-11:00	20 min.	In-Situ Data Analytics - Exploring Simulations during Runtime	Christian Gscheidle, Fraunhofer SCAI
11:00-11:30	30 min.	Centres of Excellence for HPC Applications within the New EU R&I Programme Horizon Europe	Claudio Scalese, EuroHPC Joint Undertaking
11:30-11:45	15 min.	FPGAs for HPC workloads: The Why and the How	Nick Brown, EPCC
11:45-11:50	5 min.	Q&A	All EXCELLERAT speakers
11:50-11:55	5 min.	Closing of Day 2	Ralf Schneider, HLRS

Table 5: Agenda of Conference Day 2, 17th May 2022

The conference was well-received and several participants asked for the recordings. The videos from the event were published via a playlist on the YouTube channel of FocusCoE [29], the CoEs' Coordination and Support Action. At this stage, EXCELLERAT does not have its own account and therefore asked for support of FocusCoE. The playlist was widely distributed via social media and across the attendants of the conference. This way, WP7 made sure that the content will remain available even after the project ends.

2.2.7 Media Relations

One of the major goals of WP7 was to support the project's success with measures of public relations. EXCELLERAT did not only provide the HPC trade press with valuable content, but also reached out to industry news outlets and daily press, identifying and highlighting the added value that the Centre of Excellence for Engineering Applications could bring to the layperson. In total, the media relations activities of the project led to 34 clippings, which indicates the success of these activities, as the target of 20 was overachieved. Table 6 below lists all clippings generated with mentions of EXCELLERAT.

Aside from the general press release introducing the project and a couple of interviews, the team wrote a press release highlighting how EXCELLERAT could use its tools (in this case the data workflow platform) to support COVID-19 related research. This press release was published in the end of November in German by SSC and on 1 December 2020 in English by the EXCELLERAT press office. This release generated 13 clippings, in daily press, HPC, science and trade press.

A final press release wrapping up the achievements of EXCELLERAT will be sent out after the project end, which might generate additional media coverage.

Source	Release Date	Channel	Link
Primeurmagazine	October 2018	Online/ Video	http://primeurmagazine.com/weekly/AE-PR-11-18-85.html (not available anymore due to the death of the editor in chief and thus closing of this medium)
GCSnews	October 2018	Online	https://www.gauss-centre.eu/fileadmin/user_upload/PR_News/2018/Publications/GCSnews20/GCSnews_20_2018_final_sm.pdf#page=2
HPC Wire	December 12, 2018	Online	https://www.hpcwire.com/off-the-wire/EXCELLERAT-to-bring-hpc-applications-to-engineering-industry/
INSiDE	December 2018	Online / Print	https://www.hlrs.de/fileadmin/user_upload/InSiDE_16-2_ES_web.pdf#page=7
IDW	December 3, 2018	Online	https://nachrichten.idw-online.de/2018/12/03/expert-panel-on-the-future-of-hpc-in-engineering/
Innovations Report	December 3, 2018	Online	https://www.innovations-report.de/html/berichte/veranstaltungen/live-chat-zur-zukunft-von-supercomputing-im-engineering.html
Innovations Report	January 30, 2019	Online	https://www.innovations-report.com/html/reports/information-technology/new-analysis-methods-

			facilitate-the-evaluation-of-complex-engineering-data.html
InsideHPC	March 21, 2019	Online	https://insidehpc.com/2019/03/european-commission-funds-10-centers-of-excellence-for-hpc/
InsideHPC	January 29, 2020	Online	https://insidehpc.com/2020/04/video-competence-centres-in-hpc-their-role-in-european-innovation/
datacenter-insider.de	February 25, 2020	Online	https://www.datacenter-insider.de/deutschlands-schnellster-supercomputer-werkelt-nun-in-stuttgart-a-907780/
HPC Wire	July 6, 2020	Online	https://www.hpcwire.com/2020/07/06/qa-hlrss-bastian-koller-tackles-hpc-and-industry-in-germany-and-europe/
PRACE News	July 14, 2020	Online	https://prace-ri.eu/scientists-provide-the-first-full-view-into-an-aircraft-engine/
EPCC Newsletter	August 5, 2020	Online	https://www.epcc.ed.ac.uk/sites/default/files/newsletters/EPCC%20News%2087%20summer%202020.pdf
HLRS News	August 6, 2020	Online	https://www.hlrs.de/news/detail-view/2020-08-06/
Sicos-bw.de	August 10, 2020	Online	https://www.sicos-bw.de/news-events/news-detail/sommerinterview-nicole-prange/
HPC Wire	August 31, 2020	Online	https://www.hpcwire.com/off-the-wire/european-commission-approves-two-bsc-led-high-performance-computing-centers-of-excellence/
Sicos-bw.de	September 2, 2020	Online	https://www.sicos-bw.de/news-events/news-detail/sommerinterview-anne-bernard-bedouet/
Epeec-project.eu	November 25, 2020	Online	https://epeec-project.eu/media/news/success-story-epeec-partners-excellerat-develop-treeadapt-new-library-and-application
Böblinger Zeitung	November 27, 2020	Print	-
HPC Wire	December 1, 2020	Online	https://www.hpcwire.com/off-the-wire/excellerat-coe-supports-covid-19-related-research/
Primeurmagazine	December 1, 2020	Online	http://primeurmagazine.com/weekly/AE-PR-01-21-7.html (not available anymore due to the death of the editor in chief and thus closing of this medium)

Scientific Computing	December 2, 2020	Online	https://www.scientific-computing.com/news/european-engineering-research-centre-supports-covid-19-research
Cordis	December 2, 2020	Online	https://cordis.europa.eu/article/id/428546-excellerat-coe-supports-covid-19-related-research
It It Prof	December 3, 2020	Online	https://www.it-it-prof.de/2020/12/03/ssc-unterstuetzt-bundesinstitut-fuer-bevoelkerungsforschung-bei-corona-berechnungen/
Software Journal	December 3, 2020	Online	https://www.software-journal.de/2020/12/03/ssc-unterstuetzt-bundesinstitut-fuer-bevoelkerungsforschung-bei-corona-berechnungen/
HightechBox	December 3, 2020	Online	https://www.hightechbox.de/2020/12/03/ssc-unterstuetzt-bundesinstitut-fuer-bevoelkerungsforschung-bei-corona-berechnungen/
IndustrieBox	December 3, 2020	Online	https://www.industriebox.de/2020/12/03/ssc-unterstuetzt-bundesinstitut-fuer-bevoelkerungsforschung-bei-corona-berechnungen/
TechnologieBox	December 3, 2020	Oline	https://www.technologiebox.de/2020/12/03/ssc-unterstuetzt-bundesinstitut-fuer-bevoelkerungsforschung-bei-corona-berechnungen/
Cordis	December 31, 2020	Online	https://cordis.europa.eu/article/id/428675-smart-platform-for-predicting-covid-19-healthcare-system-demands?WT.mc_id=exp
Les Echos	January 5, 2021	Online	https://www.lesechos.fr/idees-debats/sciences-prospective/le-superordinateur-allemand-contre-le-covid-19-1278232
EuroCC SLING Newsletter	March 30, 2021	via e-mail	-
ITmag-dz.com	April 26, 2021	Online	http://www.itmag-dz.com/2021/04/26/le-super-ordinateur-allemand-contre-le-covid-19/
HPC Wire	July 6, 2021	Online	https://www.hpcwire.com/2020/07/06/qa-hlrss-bastian-koller-tackles-hpc-and-industry-in-germany-and-europe/
BigDataInsider	February 8, 2022	Online	https://www.bigdata-insider.de/sicos-bw-setzt-auf-eu-projekte-a-1092980/

Table 6: List of media clippings

3 Collaboration

3.1 Introduction

An efficient use of EU funding resources and a customer-oriented development of HPC services for the field of engineering requires a well-planned and continuously maintained collaboration network. EXCELLERAT has closely cooperated with other partners involved in European and national research projects and initiatives to identify common issues in the field of HPC and to avoid investments into redundant activities.

During the first half of EXCELLERAT a large number of new collaboration activities were initiated and led to an intensive and successful exchange of tools, services and experience. The successful collaboration was continued in the second half of the project, leading to mutual benefits for all collaboration parties.

In the second year of the CoE, a collaboration success story template summarising the efforts and results of the collaborations was introduced to monitor the achievements within EXCELLERAT. The collection of the success stories was continuously extended and supplemented with the description of further collaboration activities in the last year. A selection of success stories is exemplarily shown in the next section. The success stories contributed considerably to the monitoring of on-going collaborations and to the motivation of additional collaborations. Since the summary of collaboration activities in Deliverable D7.4 [7], new collaboration has been established, which considerably expanded the collaborative network. In total, the EXCELLERAT partners cooperated in 45 projects, which are summarised in Table 7 and are described in more detail in the Annex 3 (Table 12 to Table 23).

As part of the FocusCoE platform, EXCELLERAT have already intensively cooperated with FocusCoE [30], EoCoE [31], POP2 CoE [32], Max CoE [33], ChEESE CoE [34], HiDALGO CoE [35] and CompBioMed CoE [36] to synergistically define strategies for extreme scale applications in the EU HPC Ecosystem. Besides the activities within the FocusCoE project, the EXCELLERAT project partners have a large number of existing and newly acquired collaborations with European and national projects, companies and dedicated research groups.

To further extend and maintain the collaboration network beyond the EXCELLERAT CoE, future potential partners are constantly identified and the EXCELLERAT partners are continuously establishing new cooperation activities that can still be maintained after the project end. To attract potential industrial customers and collaboration partners, information about the EXCELLERAT services has been disseminated in close collaboration with Task 7.1 (Dissemination and Communication).

Project Partner	Collaboration Project
USTUTT	FocusCoE, HiDALGO CoE, CATALYST, CRESATA, bwWisu, bwWisu2
UEDIN	CompBioMed CoE, CompBioMed2 CoE
CINECA	MAX2 COE, ETP4HPC, I4MS ICT, Prace Preparatory Access, ChEESE CoE, Hi-Fi Turb, STREAmS, PAinG-Flow
SICOS BW	RECOM SERVICES, OPTIMA PHARMA
KTH	EPiGRAM-HS, RIKEN, Scania, SeRC, FLOW, “Dong” Condition, AVM
ARCTUR	DIH HPC5
CERFACS	MMG, AVBP, CVT, EPEEC, POP2 CoE, EPI

BSC	POP2 CoE, EoCoE
FRAUNHOFER	ViPriA, VMAP, MADESI
TERATEC	POP2 CoE, FocusCoE
RWTH	SFB TRR40, ENODISE, INVENTOR, POP2 CoE
SSC	HLRS pilot project, hydrograv

Table 7: Overview of the projects collaborating with EXCELLERAT

3.2 Success Stories

In the second half of the EXCELLERAT CoE's runtime, success stories summarising the efforts and results of the completed and ongoing collaborations were created. The success stories have served, first of all, as an internal monitoring system to regularly track the status of the collaborations' achievements. In addition, the internal success stories serve to identify projects that offer services and unique values which can potentially attract new stakeholders for EXCELLERAT CoE.

Below, an example of a collaboration success story is given:

KTH – SeRC Collaboration

Partner:	**Name of the Collaboration Project:**	
KTH	SeRC	
Collaboration Partner:	**Related WP:**	**Time Frame:**
Swedish e-Science Research Centre	WP2, WP3	Feb – Dec 2020

Objectives:

The Swedish e-Science Research Centre is a national e-science initiative dedicated to provide e-infrastructure support and to improve important e-science software on future HPC platforms. Collaboration between EXCELLERAT and SeRC is concentrated on improving the performance of the NEK5000 program and getting NEK5000 ready to run on future hardware, particularly new GPU systems.

Most Important Results:

The collaboration between EXCELLERAT and SeRC began with updating NEK5000 using OpenACC directives to enable running on NVIDIA GPUs. This has been completed and the results are shown below. After profiling the OpenACC version it was found that the directive approach was creating some inefficient small kernels. Merging some kernels by re-writing them in CUDA, significantly reduced their total runtime. Also, as part of the profiling work, several routines were found to have significant bank conflicts when certain input was used. When these were removed the duration of the affected kernels improved by around 20%. In addition to the OpenACC version, an OpenMP version using GPU offload has been created to enable NEK5000 to run on AMD GPUs. The OpenMP version has currently a similar performance as the OpenACC version.

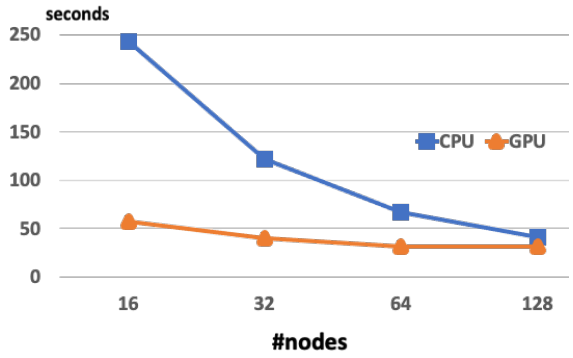

Figure 6: Pipe simulations on JUWLES Booster at Jülich Supercomputing Centre (JSC), comparing OpenACC/CUDA version and CPU version (1 nodes has a 48 core AMD EPYC and 4 A100 GPUs)

In addition to the internal success stories focused on collaboration, more comprehensive, publicly available success stories, as described in section 2.2.3, were created. The more detailed success stories especially summarise the results and advantages of the joint work and outlines the unique value and services resulting from the collaboration. As such, they support the dissemination of the services offered by EXCELLERAT, e.g., via the website or social media channels. In Annex 4, the publicly available success story of the already mentioned KTH – SeRC collaboration is given as an example.

4 Community Building

As a reminder, the goal of this activity was twofold: first, to ensure that EXCELLERAT is recognised by developers and users of engineering applications as a new key player in their ecosystem for Exascale codes in engineering, and second to link EXCELLERAT and its activities to the communities of academics and industrial users and developers, who are potential customers of EXCELLERAT's services.

As described in the D7.4 [7], the strategy decided during the EXCELLERAT AHM in Bologna (November 2019) was to monitor the EXCELLERAT community building efforts on three main levels: the initial level is the initial core of the Community (i.e. the EXCELLERAT consortium partners), the second level is constituted by the communities around the reference applications or the satellite codes which are hosted by the project (this is mainly the HPC community), finally the third level brings together all the associated partners (mainly via the Interest Groups) and all the industrial partners, the potential users/clients, the other CoEs and the general public.

4.1 Implementation

The map in Figure 7 places in a grid different types of stakeholders with their respective importance and scaled with the level of power/interest. This map was created at the beginning of the project, and continuously updated, with the aim of visualising the stakeholders concerned by EXCELLERAT and our community building actions.

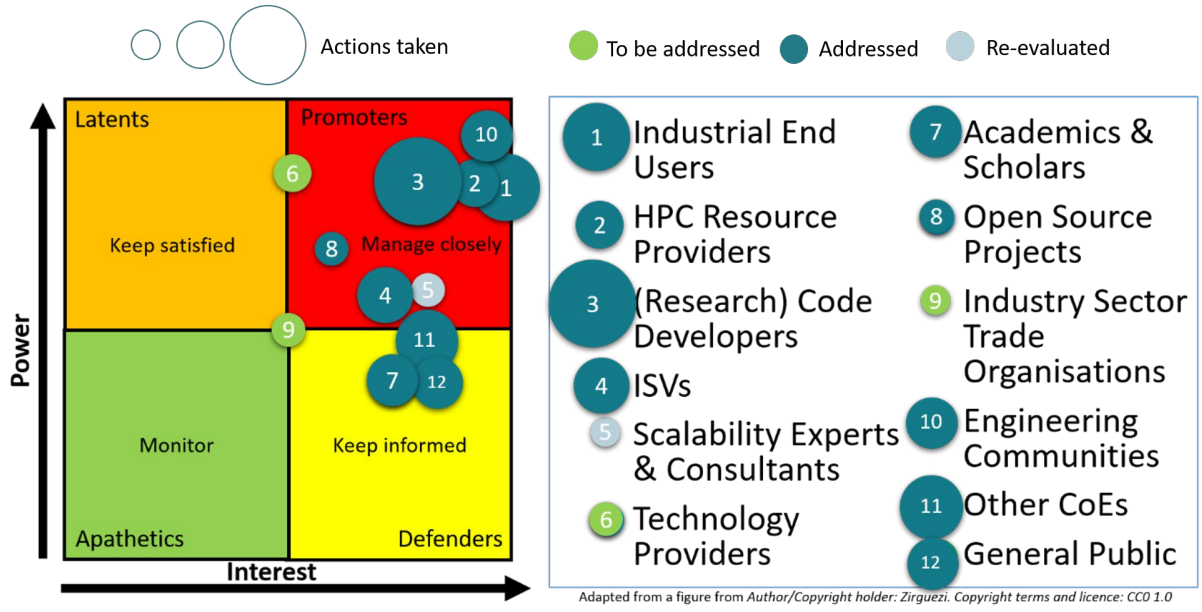

Figure 7: EXCELLERAT stakeholders map and actions. (The size of the circles on the map is proportional to the number of achieved actions. The various colours are explained in the following paragraph)

This map in Figure 7 allowed EXCELLERAT to target the most important stakeholders to ensure community building with them. All stakeholders were initially considered (see the initial map in Figure 8) before some refinements were done during the project.

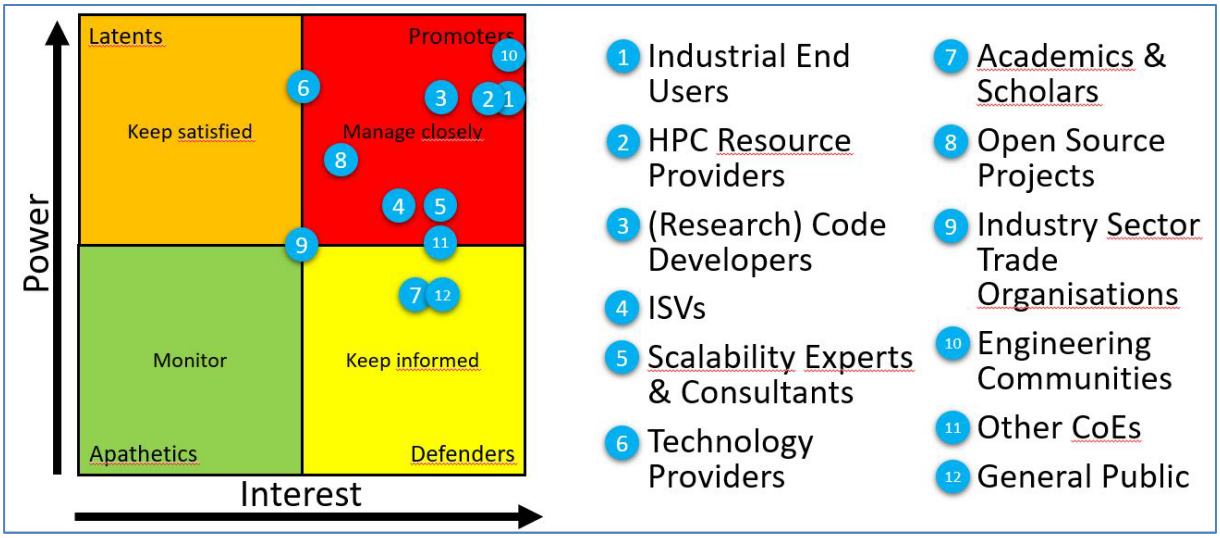

Figure 8: EXCELLERAT's initial stakeholder map before targeted actions

The updated map in Figure 7 highlights that the main targets of EXCELLERAT have been successfully reached. There have been many various events since D7.4, which was submitted at end of 2020. The five main reached targets (i.e. the ones with the most opportunities to interact and directed towards the priority stakeholders for EXCELLERAT) were:

1. For the Research code developers (n°3), 9 activities:
   - the SC20 side-event talk in November 2020,
   - the School on "Numerical methods for parallel CFD" in December 2020 at CINECA,
   - the Digital CoEs workshop (technical joint workshop) in January 2021,
   - the Fortran webinar on 04 May 2021, a talk at ISC2021 in June 2021,
   - a Mini symposium on load balancing at PASC2020, July 2021,
   - a KER ESS seminar with HRB experts in October 2021,
   - a presence at the PRACE virtual booth and presentation at SC21 in November 2021,
   - the School on "Numerical methods for parallel CFD" Dec2021 at CINECA
2. For the Industrial End users (n°1), 4 activities:
   - the SC20 side-event talk in November 2020,
   - ISC2021 in June 2021,
   - a presentation at Teratec Forum June 2021,
   - a booth and several talks at NAFEMS2021 World Congress in October 2021
   - a presence at the PRACE virtual booth and presentation at SC21 in November 2021
3. For the Academics and scholars (n°7), 4 activities:
   - the School on "Numerical methods for parallel CFD" December 2020 at CINECA,
   - a Session at the EuroHPC Summit Week March 2021 with FocusCoE,
   - the School on "Numerical methods for parallel CFD" December 2021 at CINECA
   - and a Session at the EuroHPC Summit Week March 2022 with FocusCoE
4. For the other CoEs (n°11), 4 activities:

- the School on "Numerical methods for parallel CFD" December 2020, at CINECA,
- the Digital CoEs workshop (technical joint workshop) January 2021,
- the Session at the EuroHPC Summit Week March 2021 with FocusCoE,
- the School on "Numerical methods for parallel CFD" Dec2021 at CINECA

5. For the General public (n°12), 4 activities:
   - Podcast #1 “What is the HPC?” February 2020,
   - Podcast #2 “Why do aeronautics benefit from HPC simulations?” November 2020,
   - Podcast #3 “How to Improve Autonomous Vehicles with Supercomputer Simulations?” August 2020,
   - Podcast #4 “How can simulations make aircrafts more environmentally friendly?” June 2021

In parallel, during the running of EXCELLERAT, we have noted that actually the stakeholder category “Scalability experts & consultants” (n°5) was a sub-category of the category “Research code developers” (n°3). Therefore we decided to include them in this category, hence the grey colour on the map. For the “Technology providers” (n°6) and the “Industry Sector trade organisations” (n°9), we concluded that interacting with them would be more relevant during a second phase of EXCELLERAT, once the service portfolio and the service offerings are finalised and implemented, hence the light green colour on the map.

For the events listed above, EXCELLERAT contributed either with talks given by their researchers or by running a booth (online format since the COVID-19 outbreak), by displaying communication materials (flyers, videos, success stories) and by supporting researchers and experts from the WP6 / marketing teams who presented the EXCELLERAT outcomes and services to the visitors. EXCELLERAT WP7 also organised specific workshops and webinars, for instance the CoEs technical workshop in January 2021, the Fortran webinar in May 2021 or the KER Exploitation Strategy Seminar with the HRB experts in October 2021. In these cases, the WP7 team covered all the logistics and organisational aspects.

4.2 Work Involvement of the Interest Groups

EXCELLERAT has decided to establish the so-called Interest Groups [37], whose main objectives being the communication, monitoring and validation of the project’s overall goal, as well as the industrial and technological relevance for the user communities. The Interest Groups were structured in such a way that allows providing the viewpoints of the different actors of the Centre’s value chain: Code Developers/ISVs, Industrial End Users, Scientific Experts and Technology Providers.

The first workshop for the Interest Groups was performed and recorded at the beginning of November 2019. The agenda for this meeting is presented in Table 8 below.

Topic
Introduction
Role of the Interest Groups in EXCELLERAT
Presentation of the Project (Overview of EXCELLERAT)
Presenting our new HPC data exchange platform
Video + Work plan for Vistle (Visualisation)
Presentation of the BigWhoop compression library
First Preview of the Service Portal
Questions and Advice
Summary

Table 8: IG Webinar Agenda

The purpose of this meeting was to give the IG an overview about the recent results of EXCELLERAT and the project as well as integrating them into the EXCELLERAT ecosystem. Different IG were considered, including the following:

- ISVs (offering software and service in the domain of civil engineering)
- Software developers (in academia and in industry), who contribute to the development of the EXCELLERAT application codes (or similar applications)
- Users (from academia and industry), who are interested in making sure that the future applications development's take their requirements into account
- Trade unions, who may act as an interface between the application developers and the end users, as for example.

The IG workshop facilitated the communication with the IG members, as they understood even better the purpose and the use of EXCELLERAT. The members were regularly notified of projects and (digital) events of potential interest for them.

The second IG seminar took place virtually on June 26, 2020. In this meeting, the Interest Groups were updated on EXCELLERAT's activities and introduced to the improved EXCELLERAT service portal. This was helpful, since they could provide feedback from an actual user's perspective. The final IG meeting was incorporated to the EXCELLERAT Conference, as described in section 2.2.6, since the topics of the talks provided by WP3 were originally selected by the Interest Groups and all of them were invited to the conference. Two of the Interest Groups members were keynote speakers in the listed programme.

Furthermore, the IG members were updated for example via the podcast episodes and newsletter issues, which they received via the mailing list. In 2021, the Interest Groups was further extended by two new members: Constelcom and "Falquez, Pantle and Pritz GbR" (Nuberisim). Through the IG, EXCELLERAT has been able to develop and adapt according to the important advice given by the Groups. Further information on future plans for the IG and outreach activities related to training and the service portal can be found in D5.7 [5].

5 Standardisation

5.1 Identification

EXCELLERAT focuses on the use of HPC for engineering purposes. The final product is therefore a high-fidelity simulation service adapted to the industrial needs. All high-tech products must cross the "chasm of acceptation" and HPC simulation is not an exception:

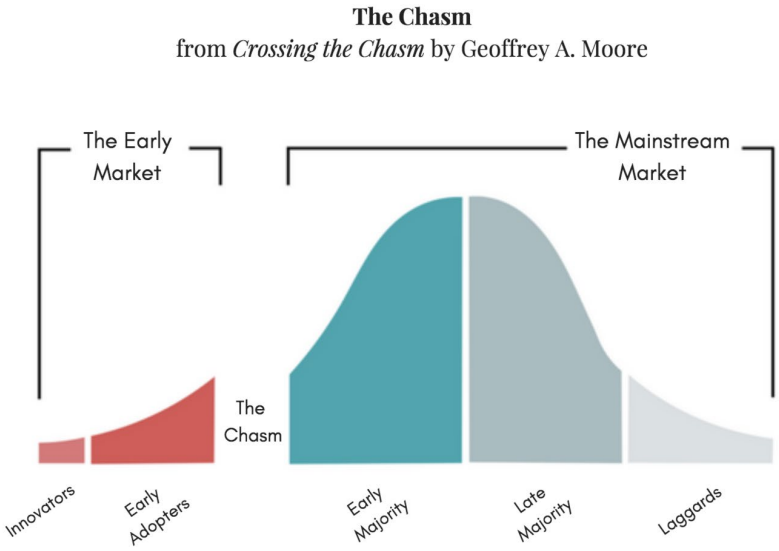

Figure 9: The "crossing the chasm" point of view

From a "crossing the chasm" point of view, the vast majority of HPC uses for engineering is, nowadays, laying around the chasm. Some bleeding edge research applications are done by the Early Adopters, usually through a PhD contract or a small bilateral contract. Many laboratories also have "industrialisation" programs to cross the chasm. A little part of their applications has already overcome the chasm with large scale usage by the Early Majority of engineers. However, the situations in which the HPC is a validated and accepted part of the design process are still very rare for now. The "standardisation" effort of EXCELLERAT is about conquering this Early Majority.

Indeed, the challenges particularly to HPC, namely Crashes, Performances and Sustainability, are three potential showstoppers on the road to acceptance. This is where the danger comes from when moving from tens to thousands HPC runs per year.

5.2 Elaboration

The task 7.2 "Standardization" addressed the challenges of Crashes, Performances in production and Sustainability using various approaches.

Concerning Crashes and Performances in production, a worked example showed how to make use of the simulation logs accumulated during a year's worth of simulation. This worked example also showed that advanced data analysis such as Principal Component Analysis and clustering were needed to make sense of this dataset. This became later the material for the first EXCELLERAT white paper.

During this period, one of our industrial partners stressed the fact that handling a campaign of simulations on the HPC clusters was a repetitive task, limited to users trained on HPC submission protocols. This was apparently a strong bottleneck linked to human resources - which is much more expensive than HPC computer resources. A lightweight tool “Lemmings” [38] to ease the submission of “standardised” workflows of the type “compute until condition is reached” was therefore developed by EXCELLERAT and is now in production.

Concerning sustainability, moving a code to a production level means a sharp increase of support. As a consequence, either the cost of a support action is decreased dramatically, or the software community will collapse under the support action. Various aspects of the technical debt of a research code were investigated within EXCELLERAT.

First, a versioning strategy [39] complying with the needs of companies on a research code was proposed as a baseline. Indeed, a good versioning strategy can avoid many misunderstandings and remove some irrelevant support actions. The proposed versioning standard addresses the particular situation of a research code, where durable and stable versions for production must coexist with frontier simulations using the very latest version. In a second time, effort was put on helping software communities to have a clean, homogenously written codebase. For this purpose, the linting code Flinter was created. This tool helps developers to visualise various metrics on the codebases, starting with the coding quality (a subjective concept that had to be customisable).

To illustrate the concept of Flinter, the following Figure 10 is a partial scan of the tools inside EXCELLERAT’s core code AVBP. The smallest circles are the lowest level subroutines. These circles are aggregated by files, then by folders. The largest circle is the full codebase folder, where the analysis was done.

The size of each circle is proportional to the number of lines of code. The colour of each circle shows how the code inside meets the coding standard expected by the team.

This view exhibits the nested aspect of the codebase. Two large files are highlighted in pink, with plenty of small purple dots. This means that they diverge from the expected standard. A quick glance inside showed that these files where copy-pasted in their original F77 formatting, and were similar to versions of the legacy CHEMKIN library.

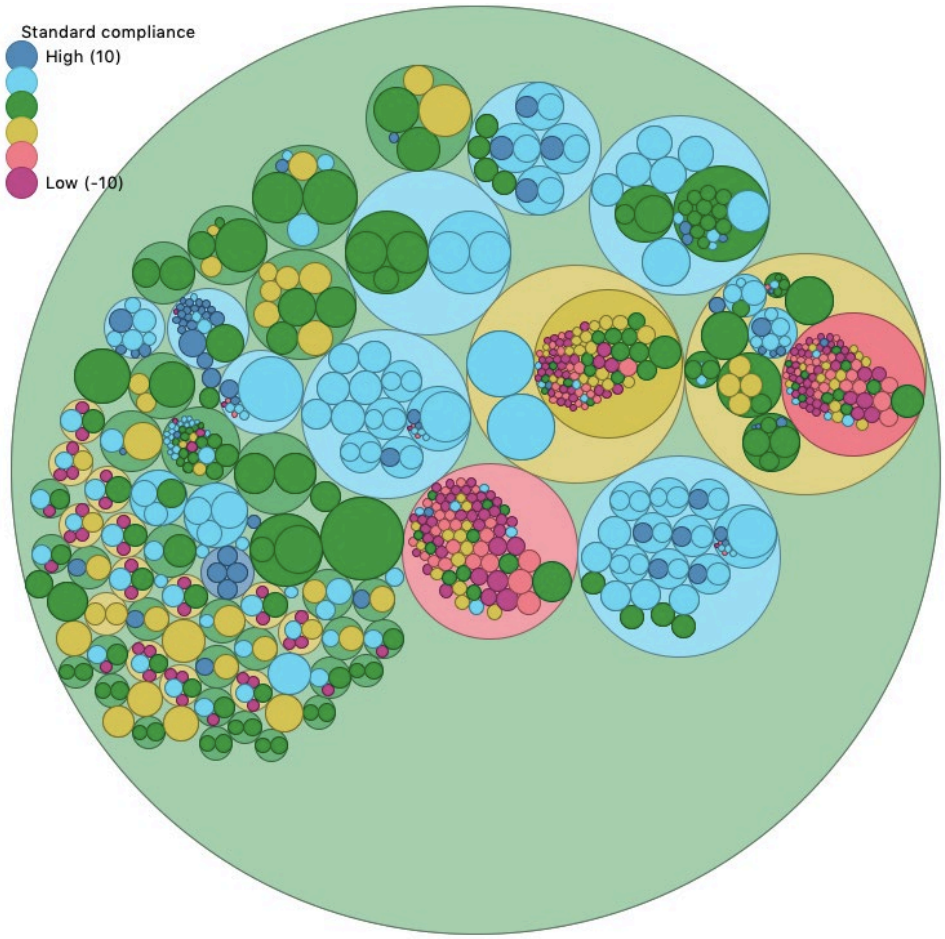

Figure 10: Visualisation of the codebase of an HPC high fidelity software, coloured by code compliance to its internal standard, using the EXCELLERAT tool Flinter

While working on Flinter, the actors of EXCELLERAT contributed to the open-source project Lizard [40] by adding support to the FORTRAN Language. Lizard allows to compute the complexity of codes at the subroutine level. With this contribution, EXCELLERAT gave to the community a way to monitor the programming complexity of all software in HPC, independent of the language.

5.3 Diffusion

The first white paper of EXCELLERAT proposed an in-depth analysis of what can be done at the end of a design simulation campaign on HPC resources at an industrial scale [12], particularly regarding what can be learned from crashes and actual performances during production.

As many of the high-fidelity software featuring both good performances and physical models are written in Fortran, a language limited to a relatively small community, EXCELLERAT hosted an advanced seminar on High-Performance Computing with Fortran in 2021, which engaged more than 100 advanced programmers.

On the one hand, contribution to International standards revealed to be not really suited to the EXCELLERAT activity, because High-Performance Computing is a niche where techniques and architecture change faster than the mainstream. In particular, software shows a very long

lifespan (up to 25 years in the core codes of EXCELLERAT) with respect to the hardware (typically three to five years of lifespan). The codes are therefore preferably partially rewritten. In this context, standards are slow to emerge.

On the other hand, many standards from mainstream computing science were investigated and adapted by EXCELLERAT to the needs of the HPC community. For example, the EXCELLERAT baseline versioning strategy cited before stems directly from the semantic versioning [41]. Concerning input validation, the json-SCHEMA [42] standard proved to be quite promising for complex input validation [43].

The tools developed within EXCELLERAT were released on open source forges like gitlab.com. Python tools like Flinter and Lemmings are parts of the Python Package Index (pypi.org) conforming to the best practices of python packages installations.

6 Conclusion

This deliverable outlined the project‘s work by WP7 to assist and to support EXCELLERAT overall. It entails the activities and results of the EXCELLERAT project regarding Communication, Dissemination, Collaboration, Community Building and Standardisation.

The following Table 9 is an overview of all deliverables produced by WP7.

Number	Title	Due	Status
D7.1	Website, Corporate Design and Template	PM 2	Submitted
D7.2	Initial Dissemination and Collaboration Plan	PM 3	Submitted
D7.3	Dissemination, Communication, Collaboration, Community Building and Standardization Report	PM 12	Submitted
D7.4	Updated Dissemination, Communication, Collaboration, Community Building and Standardization Report	PM 24	Submitted
D7.5	Final Dissemination, Communication, Collaboration, Community Building and Standardization Report	PM 42	Submitted

Table 9: Deliverables

The first milestone (Table 10) to be reached in EXCELLERAT with the help of Work Package 7 was the project Kick Off. This work package has supported this event. The second milestone MS6 can be considered as achieved once this deliverable is submitted and the project officially closes in M42.

Number	Title	Due	Status
MS1	Project Kick Off	PM 1	Done
MS6	Final Reports of all project outcomes and project close	PM 42	Done

Table 10: Milestones

Through the activities of WP7, EXCELLERAT resulted to become more visible as a Centre of Excellence for Engineering Applications, and it has increased its stakeholders' awareness to be recognised as a strong partner for collaborations and playing an important role in the community.

In the first half of the project runtime, the activities had a focus towards building the EXCELLERAT brand and mainly awareness creation – by setting up the logo, brand material, establishing all communication channels (website, blog, newsletter, Twitter account, LinkedIn account, podcast, media relations), understanding how to best approach the relevant stakeholders with planning the most suitable community building initiatives, initiating standardisation tasks and motivating partners to build a collaboration network.

In the second half, WP7 focused on disseminating the outcomes and impact of the technical work and thus leveraging them. This was undertaken, along with the ongoing activities in the scope of the continuous communications, through the development of white papers and scientific publications, with the production of 15 success stories released via all communication channels and further used as a basis for nine promotional compact e-flyers, the production of two videos (one focused on the service portal, the other one on the EXCELLERAT CoE overall), and the successful organisation of a virtual EXCELLERAT conference showcasing the results of the project to a broader audience. Eventually, these activities supported EXCELLERAT in its goal to act as a single access point to technology and expertise in the field of engineering. This is underlined by the fact that almost all WP7 KPIs targets could be achieved by M42, as well as the positive feedback received at the EXCELLERAT conference and (social) media resonance. As an outlook, the main communication channels will stay online until at least 2023 with a minimum maintenance, making sure that news beyond the project end (e.g. scientific papers currently under review) will be disseminated respectively, and that in a second project phase, the established mechanisms could be re-initiated without a major additional effort.

Following the successful implementation of a broad collaboration network in the first half of EXCELLERAT, the focus during the second half was on the efficient and targeted execution and documentation of the newly initiated cooperation activities. The efforts and achievements of completed and on-going collaboration were continuously collected and summarised using a success stories template introduced at the beginning of the second half of EXCELLERAT. To drive the awareness of the EXCELLERAT brand, unique values and services offered by EXCELLERAT were derived from these activities and promoted via the disseminated success stories mentioned above. As an outlook, the EXCELLERAT partners will continue the established cooperation activities beyond the lifetime of the project. Based on the services disseminated via the service portal, additional research and industrial partners are continuously attracted and new collaboration established. The collaboration map will be maintained beyond the end of EXCELLERAT, which will also be the basis for an efficient extension of the introduced services for a prospective second project phase of EXCELLERAT.

In terms of community building activities during the second half of EXCELLERAT, WP7 organised or attended several key events of various formats (e.g. engineering communities congress like NAFEMS World Congress 2021, technical workshops or webinars) with various audiences (see the map of stakeholders presented in section 4.1). These events ensured through their promotion, the produced material, the talks, and the discussions arising from those that EXCELLERAT is recognised by developers and users of engineering applications codes as a new key player in the ecosystem for Exascale codes in engineering. Following the COVID-19 outbreak in March 2020, all events were repeatedly postponed or went online. Therefore, WP7

created adapted communication material to be used for online promotion and for interaction with visitors to online events, hence EXCELLERAT was able to successfully take part in and advantage of the online events in replacement of the physical ones. Therefore, EXCELLERAT and its activities were able to continue to liaise with the communities of academics, industrial users and developers throughout the COVID-19 pandemic until the end of the project. This was possible thanks to the efforts put in adapting to the new ways of community building. Consequently, these communities are already now or will soon be users of EXCELLERAT's services.

The standardisation task showed that the evolution from demonstration simulations to full scale production comes with new challenges seldom addressed in the HPC community. In particular, the human time involved when scaling up the production can easily make the business unsustainable. Questions the standardisation task dealt with were:

- How do we run large simulations campaigns involving thousands of jobs on an HPC resource with a limited and non-expert pool of workers?
- How do we monitor computational waste (crashes, wrong inputs), and learn from our mistakes?
- How do we anticipate and reduce the manpower dedicated to support?

EXCELLERAT Phase 1 provided several practical solutions through best practices, tools and a white paper. Two critical fronts remain for the future: First, the concept of production workflow on HPC resources must gain maturity with applied examples for various actual customers. Second, the HPC community needs new approaches and tools to lower the technical debt of software. In the end, even if saving computing time is important, saving the human time of trained experts is of even higher value.

7 References

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Annex 1: EXCELLERAT Publications

Title	Authors	Title of the Journal/Proc./Book	DOI	Repository Link
Parallel SFC-based mesh partitioning and load balancing	Ricard Borrell, Guillermo Oyarzun, Damien Dosimont, Guillaume Houzeaux	2019 IEEE/ACM 10th Workshop on Latest Advances in Scalable Algorithms for Large-Scale Systems (ScalA)	10.1109/scala49573.2019.00014	https://arxiv.org/abs/2007.03518
Heterogeneous CPU/GPU co-execution of CFD simulations on the POWER9 architecture: Application to airplane aerodynamics	Ricard Borrell, Damien Dosimont, Marta Garcia-Gasulla, Guillaume Houzeaux, Oriol Lehmkuhl, Vishal Mehta, Herbert Owen, Mariano Vázquez, Guillermo Oyarzun	Future Generation Computer Systems	10.1016/j.future.2020.01.045	https://arxiv.org/abs/2005.05899
Performance Analysis of Complex Engineering Frameworks	Wagner, Michael und Jägersküpper, Jens und Molka, Daniel und Gerhold, Thomas	Tools for High Performance Computing 2019		https://elib.dlr.de/132767/
Improving Strong Scalability Limits of Finite Element Based Solvers	Niclas Jansson	Kyoto, The 48th International Conference on Parallel Processing (ICPP 2019)		https://www.hpcs.cs.tsukuba.ac.jp/icpp2019/data/posters/Poster7-abst.pdf
EXCELLERAT: il centro di eccellenza europeo per le applicazioni di ingegneria	Raffaele Ponzini, Francesco Salvadore, Claudio Arlandini	Analisi e calcolo		https://aec-analisiecalcolo.it/notizie/453-/
Abstract: Quantifying Uncertainties in high-fidelity Scale-Resolving Simulations of Wall Turbulence	Philipp Schlatter, Saleh Rezaeiravesh, Ricardo Vinuesa	72nd Annual Meeting of the APS Division of Fluid Dynamics		https://meetings.aps.org/Meeting/DFD19/Session/H41.8 https://frontuq19.files.wordpress.com/2019/09/frontuq19_book_of_abstracts-1.pdf
Active flow control for external aerodynamics: from micro air vehicles to a full aircraft in stall	Oriol Lehmkuhl, Adrian Lozano-Duran, Ivette Rodriguez	Conference: Fourth Madrid Turbulence Summer Workshop, 2019		https://www.researchgate.net/profile/Oriol_Lehmkuhl/publication/338281910_Active_flow_

				control_for_external_aerodynamics_from_micro_air_vehicles_to_a_full_aircraft_in_stall/links/5e0ba659299bf10bc3874ce5/Active-flow-control-for-external-aerodynamics-from-micro-air-vehicles-to-a-full-aircraft-in-stall.pdf
Exploring the Acceleration of the Met Office NERC Cloud Model Using FPGAs	Nick Brown	High Performance Computing - ISC High Performance 2019 International Workshops, Frankfurt, Germany, June 16-20, 2019, Revised Selected Papers	10.1007/978-3-030-34356-9_43	
Mastering Exascale Challenges for Engineering Applications	Bastian Koller, Ralf Schneider, Andreas Ruopp, Dimitris Liparas	Sustained Simulation Performance 2018 and 2019 - Proceedings of the Joint Workshops on Sustained Simulation Performance, University of Stuttgart (HLRS) and Tohoku University, 2018 and 2019	10.1007/978-3-030-39181-2_2	
High Performance Computing und Datenmanagement für Ingenieursanwendungen in Forschung, Mittelstand und Industrie	Bastian Koller, Ralf Luithardt	ProduktDatenJournal		https://www.excellerat.eu/wp-content/uploads/2022/05/pdj18-2_de.pdf
Effect of the Actuation on the Boundary Layer of an Airfoil at	Oriol Lehmkuhl, Ivette Rodriguez, Ricard Borrell	Direct and Large Eddy Simulation XII	10.1007/978-3-030-42822-8_41	

Moderate Reynolds Number				
Effects of the Actuation on the Boundary Layer of an Airfoil at Reynolds Number Re = 60000	Ivette Rodriguez, Oriol Lehmkuhl, Ricard Borrell	Flow, Turbulence and Combustion	10.1007/s10494-020-00160-y	
Active flow control for external aerodynamics: from micro air vehicles to a full aircraft in stall	Oriol Lehmkuhl, Adrián Lozano-Durán, Ivette Rodriguez	Journal of Physics: Conference Series	10.1088/1742-6596/1522/1/012017	http://hdl.handle.net/2117/191718
Weighing up the new kid on the block: Impressions of using Vitis for HPC software development	Nicholas Brown	30th international conference on Field-Programmable Logic and Applications (FPL)	10.1109/FPL50879.2020.00062	https://ieeexplore.ieee.org/stampPDF/getPDF.jsp?tp=&arnumber=9221613&ref=aHR0cHM6Ly9pZWVleHBsb3JlLmllZWUub3JnL2Fic3RyYWN0L2RvY3VtZW50LzkyMjE2MTM=
A Hybrid MPI+PGAS Approach to Improve Strong Scalability Limits of Finite Element Solvers	Niclas Jansson	IEEE Cluster 2020	10.1109/CLUSTER49012.2020.00041	https://ieeexplore-ieee-org.focus.lib.kth.se/document/9229577
Investigating applications on the A64FX	Adrian Jackson, Michèle Weiland, Nick Brown, Andrew Turner, Mark Parsons	Embracing Arm: a journey of porting and optimization to the latest Arm-based processors		https://arxiv.org/abs/2009.11806
Exploring the acceleration of Nekbone on reconfigurable architectures	Nicholas Brown	Sixth International Workshop on Heterogeneous High-performance Reconfigurable Computing (H2RC'20)	10.1007/978-3-030-34356-9_43	https://link.springer.com/chapter/10.1007/978-3-030-34356-9_43
An uncertainty-quantification framework for assessing accuracy, sensitivity, and	Saleh Rezaeiravesh, Ricardo Vinuesa, Philipp Schlatter	Journal of Computational Physics	https://doi.org/10.1016/j.jocs.202	https://www.sciencedirect.com/science/article/pii/S1877750322000941

robustness in computational fluid dynamics			2.101688	
It's All About Data Movement: Optimising FPGA Data Access to Boost Performance	Nick Brown, David Dolman	2019 IEEE/ACM International Workshop on Heterogeneous High-performance Reconfigurable Computing (H2RC)	10.1109/H2RC49586.2019.00006	https://ieeexplore.ieee.org/stampPDF/getPDF.jsp?tp=&arnumber=8945776&ref=aHR0cHM6Ly9pZWVleHBsb3JlLmllZWUub3JnL2RvY3VtZW50Lzg5NDU3NzY=
Spectral Element Simulations on the NEC SX-Aurora TSUBASA	Niclas Jansson	HPCAsia 2021	10.1145/3432261.3432265	https://dl.acm.org/doi/pdf/10.1145/3432261.3432265
Applying Bayesian Optimization with Gaussian Process Regression to Computational Fluid Dynamics Problems	Yuki Morita, Saleh Rezaeiravesh, Narges Tabatabaei, Ricardo Vinuesa, Koji Fukagata, Philipp Schlatter	Journal of Computational Physics	https://doi.org/10.1016/j.jcp.2021.110788	
UQit: A Python package for uncertainty quantification (UQ) in computational fluid dynamics (CFD)	Saleh Rezaeiravesh, Ricardo Vinuesa, Philipp Schlatter	Journal of Open Source Software (JOSS)	https://doi.org/10.21105/joss.02871	https://joss.theoj.org/papers/10.21105/joss.02871
On Numerical Uncertainties in Scale-Resolving Simulations of Canonical Wall Turbulence	Saleh Rezaeiravesh, Ricardo Vinuesa, Philipp Schlatter	Computer and Fluids	https://doi.org/10.1016/j.compfluid.2021.105024	https://www.sciencedirect.com/science/article/pii/S0045793021001900
Towards multifidelity models with calibration for turbulent flows	Saleh Rezaeiravesh, Ricardo Vinuesa, Philipp Schlatter	14th World Congress on Computational Mechanics (WCCM) and ECCOMAS Congress, 2021	10.23967/wccm-eccomas.2020.348	https://www.scipedia.com/public/Rezaeiravesh_et_al_2021a
Towards the Large-Eddy Simulation of a full engine: Integration of a 360	Carlos Pérez Arroyo, Jérôme Dombard, Florent Duchaine, Laurent Gicquel,	Journal of the Global Power and Propulsion Society	https://doi.org/10.33737/jg	https://journal.gpps.global/Towards-the-Large-Eddy-Simulation-of-a-

azimuthal degrees fan, compressor and combustion chamber. Part I: Methodology and initialisation	Benjamin Martin, Nicolas Odier, Gabriel Staffelbach		pps/133115	full-engine-Integration-of-a-360-azimuthal,133115,0,2.html
Towards the Large-Eddy Simulation of a full engine: Integration of a 360 azimuthal degrees fan, compressor and combustion chamber. Part II: Comparison against stand-alone simulations	Carlos Pérez Arroyo, Jérôme Dombard, Florent Duchaine, Laurent Gicquel, Benjamin Martin, Nicolas Odier, Gabriel Staffelbach	Journal of the Global Power and Propulsion Society	https://doi.org/10.33737/jgpps/133115	https://journal.gpps.global/Towards-the-Large-Eddy-Simulation-of-a-full-engine-Integration-of-a-360-azimuthal,133116,0,2.html
Hierarchical Multifidelity Models with Calibration for Turbulent Flows	Saleh Rezaeiravesh, Timofey Mukha, Ricardo Vinuesa, Philipp Schlatter	9th Conference on Computational Methods in Marine Engineering (Marine 2021)		https://congresos-cimne.cimne.upc.edu/cimne/custom/Congresos/Congreso_ID_12/Abstract/A_IDC12_266.pdf
Bayesian Optimisation with Gaussian Process Regression Applied to Fluid Problems	Saleh Rezaeiravesh, Yuki Morita, Narges Tabatabaei, Ricardo Vinuesa, Koji Fukagata, Philipp Schlatter	iTi 2021: Progress in Turbulence IX	https://doi.org/10.1007/978-3-030-80716-0_18	https://link.springer.com/chapter/10.1007/978-3-030-80716-0_18
Cache-aware Sparse Patterns for the Factorized Sparse Approximate Inverse Preconditioner	Sergi Laut, Ricard Borrell and Marc Casas	ACM International Symposium on High-Performance Parallel and Distributed Computing (HPDC'21)	https://doi.org/10.1145/3431379.3460642	https://dl.acm.org/doi/abs/10.1145/3431379.3460642
Accelerating advection for atmospheric modelling on Xilinx and Intel FPGAs	Nick Brown	IEEE International Conference on Cluster Computing (CLUSTER)	10.1109/Cluster48925.2021.00113	https://ieeexplore.ieee.org/stampPDF/getPDF.jsp?tp=&arnumber=9556074&ref=aHR0cHM6Ly9pZWVleHBsb3JlLmllZWUub3JnL2Fic3RyYWN0L2RvY3VtZW50Lzk1NTYwNzQ=

Towards adaptive simulations of turbulent wings at high Reynolds numbers	Fermin Mallor, Alvaro Tanarro, Nicolas Offermans, et.al.	13th International ERCOFTAC Symposium Engineering, Turbulence, Modelling and Measurements (ETMM13)		https://arxiv.org/pdf/2108.12317.pdf
Porting in-compressible flow matrix assembly to FPGAs for accelerating HPC engineering simulations	Nick Brown	IEEE Technical Consortium on High Performance Computing (IEEE TCHPC)	10.1109/H2RC54759.2021.00007	https://ieeexplore.ieee.org/abstract/document/9651274/references#references
On the Characteristics of the Super-Critical Wake behind a Circular Cylinder	Ivette Rodriguez, Oriol Lehmkuhl	Fluids 2021	10.3390/fluids6110396	https://www.mdpi.com/2311-5521/6/11/396
Dynamic load balance of chemical source term evaluation in high-fidelity combustion simulations	Guillem Ramirez-Miranda; Daniel Mira; Eduardo J. Pérez-Sánchez; Anurag Surapaneni; Ricard Borrell; Guillaume Houzeaux; Marta Garcia-Gasulla	Computers and Fluids		May 2022: in revision process, to be released soon
Scalability Evaluation of the CFD Solver CODA on the AMD Naples Architecture	Michael Wagner	Sustained Simulation Performance 2021		Will be published in autumn 2022
Communication-aware Sparse Patterns for the Factorized Sparse Approximate Inverse Preconditioner	Sergi Laut, Ricard Borrell, Marc Casas	Proceedings of the 31st International Symposium on High-Performance Parallel and Distributed Computing (Minneapolis, MN, USA) (HPDC '22)	https://doi.org/10.1145/3502181.3531472	in press
Shape-feature approach for locally accurate prediction of CFD simulation results	Daniela Steffes-lai, Rodrigo Iza-Teran, Christian Gscheidle, Jochen Garcke	NAFEMS Seminar on Machine Learning und Artificial Intelligence in der Strömungsmechanik		not yet published

		und der Strukturanalyse		
Explorative In-situ Analysis of Turbulent Flow Data Based on a Data-Driven Approach	Christian Gscheidle, Jochen Garcke	The 8th European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS Congress 2022)		not yet published
Preparing a Fortran legacy code for the upcoming exascale architectures	Joeffrey Legaux, Gabriel Staffelbach	Interdisciplinary challenges towards exascale fluid dynamics II, The 8th European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS Congress 2022)		not yet published
Estimating uncertainty of low- and high-order turbulence statistics in wall turbulence	Saleh Rezaeiravesh et al.	12th International Symposium on Turbulence and Shear Flow Phenomena (TSFP12), Osaka, Japan (Online), July 19--22, 2022	tbd	to be submitted
In-situ Estimation of Statistical Uncertainties in Turbulent Flow Simulations	Saleh Rezaeiravesh, Christian Gscheidle, Philipp Schlatter, Jochen Garcke			to be submitted

Table 11: EXCELLERAT Publications

Annex 2: Communication Kit – EXCELLERAT Conference

Online Conference: Enabling Exascale potentials for engineering applications

16th May 2022, 14:00-16:35 o'clock CEST
17th May 2022, 09:00-11:55 o'clock CEST

Dear EXCELLERAT partners, we would like to invite you to join us and spread the word about the **EXCELLERAT Conference "EXCELLERAT: Enabling Exascale potentials for engineering applications",** which will be held virtually via Webex on Monday, 16th May 2022, 14:00-16:35 o'clock CEST, and Tuesday, 17th May 2022, 09:00-11:55 o'clock CEST. You already received the calendar invitation last week. To ensure we reach a broad audience, we would like to ask for your help in promoting the event through social media, on your websites, via your institution's or related projects' newsletters or via email. In this document (and attached) you will find visual material, as well as some suggested texts/posts to use when promoting the event. We really appreciate your support and look forward to seeing you on the 16th and 17th May!

EXCELLERAT Event Page
You can find the latest information on the EXCELLERAT Service Portal:
https://services.excellerat.eu/viewevent/61
This will be updated and completed with an agenda and more details on the speakers as we get closer to the event.
The registration page has been set up via Eventbrite in order to manage attendance and ensure the acceptance of the privacy policy.

Your Promotion via Website, Newsletter, Direct Mailing
Feel free to adapt and use this text to include in your institution's website (events section), newsletters or direct mailing.

Long version:
Join us at the virtual two-day online conference "EXCELLERAT: Enabling Exascale potentials for engineering applications" on 16th and 17th May 2022! This event will showcase the impact, innovations and tools resulting from the EU-funded EXCELLERAT Centre of Excellence.
We will highlight the industrial perspective of numerical simulation and showcase EXCELLERAT's technical achievements related to its potential towards Exascale computing, scalability, accelerators and GPU computing, adaptive mesh refinement, data management, visualisation, and emerging technologies.
Our special guests will be representatives from the European Commission, the EuroHPC Joint Undertaking, Safran Aircraft Engines, and the Leonardo Labs.

Dates and times:

- Day 1: 16 May 2022, 02:00-04:35 pm CEST
- Day 2: 17 May 2022, 09:00-11:55 am CEST

Registration:
https://www.eventbrite.com/e/excellerat-enabling-exascale-potentials-for-engineering-applications-registration-317426710837

Short version:

Join us at our upcoming online conference "EXCELLERAT: Enabling Exascale potentials for engineering applications", taking place from 16 until 17 May 2022 – with special guests from the European Commission, EuroHPC Joint Undertaking, and industry companies Safran Aircraft Engines as well as the Leonardo Labs. Learn more on our Service Portal and register online.

Social Media (Twitter and LinkedIn)

The following texts and graphic elements were created for Twitter and LinkedIn, as EXCELLERAT is active on these platforms, but feel free to adapt and use them on other social platforms, such as Facebook. Please make sure to also attach your preferred visual. Ideally, all posts should be accompanied by a visual. These posts shall serve as save the date invitations and general promotion of the event, encouraging users to register. EXCELLERAT's announcements via Twitter and LinkedIn will start on Wednesday, 13th April. Further posts planned on behalf of EXCELLERAT's channels (e.g. announcing specific parts and speakers of the event) will be shared with the consortium's social media ambassadors as we get closer to the event. Furthermore, the event will be announced via our next newsletter issue in the end of April.

Accounts to be tagged:
Twitter = *@EXCELLERAT_CoE*
LinkedIn = *@EXCELLERAT*
Partners (Twitter): *https://twitter.com/i/lists/864421921299066880*

SAVE THE DATE
Twitter:

Save the date ❗

Join us at our online event "Enabling Exascale potentials for engineering applications"– with special guests from the @EU_Commission, @EuroHPC_JU, and industry companies @SAFRAN Aircraft Engines and @Leonardo_live Labs.
📅 16-17 May
➡ bit.ly/3xiTQ5t

LinkedIn:

SAVE THE DATE: Register for our EXCELLERAT online conference "Enabling Exascale potentials for engineering applications", where you can learn more about the industrial perspective of numerical #simulation and experience EXCELLERAT's technical achievements related to its potential towards Exascale computing, scalability, accelerators and GPU computing, adaptive mesh refinement, data management, visualisation, and emerging technologies.

Special guests will be representatives from the European Commission, EuroHPC Joint Undertaking and industry companies CFE-CGC Safran Aircraft Engines, and the Leonardo Labs. Stay tuned for more details!

16-17 May 2022
https://www.eventbrite.com/e/excellerat-enabling-exascale-potentials-for-engineering-applications-registration-317426710837

GENERAL PROMOTION

Twitter:

Don’t miss our online conference! Meet our special guests from industry and politics. Topics:

- **Exascale computing**
- **scalability**
- **accelerators and GPU computing**
- **adaptive mesh refinement**
- **data mgmt.**
- **visualisation**
- **emerg. Technologies**

16-17 May
bit.ly/3xiTQ5t

LinkedIn:

Don’t miss our online conference "Enabling Exascale potentials for engineering applications" in May – register now! Meet our special guests from industry and politics.

Learn more about the following topics:

- **Exascale computing**
- **scalability**
- **accelerators and GPU computing**
- **adaptive mesh refinement**
- **data management**
- **visualisation**
- **emerging technologies**

16-17 May 2022
https://www.eventbrite.com/e/excellerat-enabling-exascale-potentials-for-engineering-applications-registration-317426710837

Annex 3: Detailed Description of the Collaboration of the EXCELLERAT Partners

In the following, an overview of the existing and newly acquired collaboration of the EXCELLERAT partners is provided (Table 13 – Table 24).

Institution	Collaboration Project	Collab. Partner	Related WP/Task	Time Frame
USTUTT	CRESTA, bwWisu, beWisu2	HLRS	WP4/T4.2	Ongoing - 2021
	Description: Development of the visualization tool Vistle (the VISualization Testing Laboratory for Exascale computing, is an extensible software environment that integrates simulations on supercomputers, post-processing and parallel interactive visualization).			
	FocusCoE	SCAPOS AG	All	Nov 2019 - Nov 2021
	Description: Representation of EXCELLERAT in the FocusCoE Activities, participation in the FocusCoE project board.			
	HIDALGO	ARH, ATOS, BUL, DIALOGIK, ECMWF, HLRS, ICCS, Know-Center, MOONSTAR, MK, PLUS, PSNC, SZE	WP3, WP4	Nov 2019 - Nov 2021
	Description: Evaluation and optimization of the HIDALGO CFD codes. Definition of optimal simulation parameters. Examination and improvement of the parallelization. Optimization of pre-processing, geometry preparation and mesh generation.			
	CATALYST	SCAPOS AG	WP4	Nov 2019 - Nov 2021
	Description: Exploration of Synergies in the area of Data Management, Data Analytics.			
	No name	ENCI, CEA, Airbus	All	Ongoing
	Description: Identify potential R&D Success stories with Airbus and Onera and work on prototypes to show the successful application of HPC to industry.			

Table 12: Detailed Collaboration USTUTT

Institution	Collaboration Project	Collab. Partner	Related WP/Task	Time Frame
UEDIN	CompBioMed CoE	UEDIN, UCL, BSC, UvA, SURFsara, Uni of Oxford, Uni of Geneve, Uni of Sheffield, CBK, UPF, LifeTec Group, Acellera, Evotec UK	All	Oct 2016 – Sep 2019

		Ltd, Bull (Atos), Janssen		
	Description: WP Leader for Sustainability and Innovation, Porting Applications and general User Support on local HPC systems, Co-author of two "HPC for Medics" courses.			
	CompBioMed2 CoE	UCL, BSC, UvA, SURFsara, Uni of Oxford, Uni of Geneve, Uni of Sheffield, CBK, UPF, Acellera, Evotec UK Ltd, Bull (Atos), Janssen, LRZ, Argonne and Rutgers	All	Oct 2019 – Sep 2023
	Description: Porting Applications and general User Support on local HPC systems, bringing in new Software Solutions, running webinar series in collaboration with VPH.			

Table 13: Detailed Collaboration UEDIN

Institution	Collaboration Project	Collab. Partner	Related WP/Task	Time Frame
CINECA	MAX2 COE	CNR, SISSA, ICN2, E4, JULICH, EPFL, BSC, ETHZ, KTH, UNESCO (Fr), Cloudweavers	WP2, WP4, WP6, WP7	Dec 2018 - Nov 2021
	Description: Adaptability and Auto-tuning: Making performance available to end users. Exascaling and co-design technologies: Identify and address the gaps towards the pre- and Exascale. High level domain-specific support.			
	Prace Preparatory Access	ESI, Intel	WP3	Ongoing
	Description: HPC Performance Improvement for OpenFOAM linear solvers, creating an interface to external solver libraries such as PETSc/Hypre thus providing to the users a greater choice and flexibility when solving their cases. Increase the performances, in term of execution time, for very large test-cases (at least 50 M of cells) running on massively parallel cluster (order of thousands of cores).			
	ChEESE CoE	BSC, INGV, IMO, ETH, HLRS, CINECA, TUM, LMU, university Malaga, NGI, IPGP, CNRS, ATOS	WP3	2019 - 2022
	Description: Improve performance of linear solver algebra for simulation of solid earth. Optimization of ASHEE (Multiphase fluid dynamic model conceived for compressible mixtures composed of gaseous components and solid particle phases, based on OpenFOAM), bringing in new Software Solutions, running webinar series in collaboration with VPH.			

	Hi-Fi Turb	NUMECA, ERCOFTAC, DLR, Cenaero, CERFACS, Imperial College London, ONERA, ANSYS, DASSAULT AVIATION, UCLouvain, CINECA, UNIBG, BSC, Safran, TSAGI	WP3	2019 - 2022
	Description: Improving the capabilities of models for complex fluid flows, offers the potential of reducing energy consumption of aircraft, cars, and ships, with consequent reduction in emissions and noise of combustion based engines.			
	STREAmS	Sapienza University of Rome	WP3, WP4	2019-2022
	Description: Development of compressible turbulence code for canonical flows. The activity focused on porting to multi-GPU architectures, and code optimization. The code is called STREAmS and is provided to the community as open-source. A journal paper has been published in Computer Physics Communications.			
	PAinG-Flow	Sapienza University of Rome	WP3, WP4	2019-2022
	Description: The activity involved the porting to GPU of an incompressible turbulence code with particles modeled two-way using an ERPP algorithm. The porting, even if not fully completed, is in an advanced stage and will allow us to study particle configurations that are particularly computationally demanding and for which GPUs can offer considerable advantages.			

Table 14: Detailed Collaboration CINECA

Institution	Collaboration Project	Collab. Partner	Related WP/Task	Time Frame
SICOS BW	RECOM SERVICES	HLRS	WP4/T4.2	2019
	Description: With the help of the 3D simulation software RECOM-AIOLOS, specially designed by RECOM for industrial furnaces, the combustion and pollutant formation processes of the plant process can be mapped in virtual reality without any effects on the running operation time, for very large test-cases (at least 50 M of cells) running on massively parallel cluster (order of thousands of cores).			
	OPTIMA PHARMA	HLRS	WP4/T4.2	2018
	Description: By using simulation and visualization technologies, OPTIMA pharma visualizes the air flows in clean room systems as an essential quality factor. The medium-sized company thus minimizes the			

	risk of planning errors, accelerates the planning process and achieves cost savings.

Table 15: Detailed Collaboration SICOS BW

Institution	Collaboration Project	Collab. Partner	Related WP/Task	Time Frame
KTH	EPiGRAM-HS	EPCC, ETH, FRAUNHOFER, CRAY, ECMWF	WP2, WP3	2018 - 2019
	Description: Modernization/refactoring of Nek5000, targeting heterogeneous systems.			
	RIKEN	RIKEN	T3.2, T4.2	2016 - 2021
	Description: Methods for extreme-scale industrial CFD, including in-situ techniques, dynamic load balancing methods and adaptive mesh refinement.			
	Scania	Scania	N/A	2015 - 2021
	Description: Optimization of industrial CFD use cases using ISV codes; benchmarking of various hardware options.			
	SeRC	KTH	WP2, WP3	on-going
	Description: National large-scale e-Science initiative and national project dedicated to improve important e-science software on future HPC platforms, including Nek5000.			
	FLOW	KTH	WP2	on-going
	Description: KTH is home of the internationally recognised Linné FLOW Centre which focuses on fundamental aspects of fluid dynamics.			
	"Dong" Condition	Linköping University	WP2	May 2021-on-going
	Description: As an option for avoiding the "reverse-flow" issue in Nek5000, the so-called Dong condition can be applied at the outlet boundaries. In practice, this boundary condition has been found to work for different simulations of flows involving the convection of vortical structures at the outlet. Through a collaboration with Prof. Nordstrom's group, it is aimed to provide mathematical proof supported by computer simulations for the application of Dong condition to turbulent flows.			
	AVM	Uppsala University	WP2	May 2021 – on-going
	Desicription: Stabilization of high-order numerical approaches for simulation of high-Reynolds numbers turbulent flows is necessary. In Nek5000, there are two types of spatial filtering available for this purpose. To overcome some of the drawbacks of these methods, we aim at implementing an artificial viscosity model (AVM) for stabilization as well as subgrid-scale modeling in Nek5000. This will be pursued through a collaboration with Dr. Nazarov who is an expert on stabilization of finite-element methods. The final implementation of			

	AVM in Nek5000 will be examined for simulation of different types of turbulent flows.

Table 16: Detailed Collaboration KTH

Institution	Collaboration Project	Collab. Partner	Related WP/Task	Time Frame
ARCTUR	DIH HPC5	eXact Lab, Info.era, Sontius, Spin, Vahta, Xlab	WP6	Sep 2017 on-going
	Description: HPC5 stimulates and sustains a business growth system in technologically oriented vertical niches focusing in the Slovenia-Italy cross-border region.			

Table 17: Detailed Collaboration ARCTUR

Institution	Collaboration Project	Collab. Partner	Related WP/Task	Time Frame
CERFACS	MMG	INRIA	WP2	On-going
	Description: Use case C3U1 relies on mesh adaptation techniques developed for sequential execution by INRIA on the open source library MMG. The collaboration with INRIA dates back to 4 years as we evaluate and develop new metric methods to use MMG on complex physical cases.			
	AVBP	CORIA	WP2	2019 - 2020
	Description: CERFACS and CORIA have a long history of collaboration for CFD applications. They have worked in the past on parallel mesh adaptation techniques for incompressible flows. The current collaboration focuses on extending methods developed by CORIA to compressible flows and introducing them to AVBP.			
	CVT	GENCI	WP3	2019
	Description: CERFACS is part of the technology watch group of GENCI, the tier1 and PRACE systems manager for France. Within the CVT collaboration access and support is provided to CERFACS to port and optimize the code on new architectures. Within EXCELLERAT this concerns for now the ARM thunderx2 architecture and will be extended in 2020 to AMD Roma. This work is included in the WP3 node level and system level optimization tasks.			
	EPEEC	CERFACS	WP2, WP3	2019 - 2021
	Description: In the H2020 project, EPEEC, CERFACS developed a parallel hierarchical mesh partitioner for optimized load balancing in many core systems. Within EXCELLERAT we have extended it for load rebalancing and support for int64 required for mesh adaptation (WP2: use			

	case C3U1). Also this partitioner is required for massively many core systems and is use in the WP3 system level optimization task.			
	POP 2 COE	BSC/UVSQ	WP2, WP3	Jan 2020 - Dec 2020
	Description: Evaluation of the performance of AVBP code on the use cases using POP2 methods and tools. Identify bottlenecks and potential improvements.			
	EPI	GENCI/JSC	WP3	Jan 2020 - Dec 2020
	Description: Port and Benchmark core code in ARM technologies			

Table 18: Detailed Collaboration CERFACS

Institution	Collaboration Project	Collab. Partner	Related WP/Task	Time Frame
BSC	POP	/	WP3, T3.1	May 2019 - ongoing
	Description: Apply load balancing strategies for chemical reactions in detailed chemistry			
	EoCoE	BSC-INFIRA	WP2	2019
	Description: Using a better solver for the Poisson equation in replacement of GMRES and Conjugate Gradient			

Table 19: Detailed Collaboration BSC

Institution	Collaboration Project	Collab. Partner	Related WP/Task	Time Frame
FRAUNHOFER	ViPriA	SCALE, SIDACT, AUDI, Porsche, Volkswagen	WP4, T4.3	Oct 2019-Sep2022
	Description: The goal of the project ViPriA is the development of intelligent assistance systems based on artificial intelligence and machine learning approaches to support engineers in simulation-based, virtual product development.			
	VMAP	29 partners from 6 countries	WP4, T4.3	Sep 2017 – Aug 2020
	Description: The VMAP project will create new concepts for a universal material exchange interface for virtual engineering workflows. These concepts will be concretized in an open software standard.			
	MADESI	TU Darmstadt, Weidmüller Monitoring Systems, ZF Friedrichshafen	WP4, T4.3	Oct 2018 – Sep 2022
	Description: The analysis of sensor data of machines, plants or buildings makes it possible to detect anomalous states early and thus to avoid further damage. For this purpose, the monitoring data is searched for anomalies. By means of machine learning, anomaly detection can already be partially automated.			

Table 20: Detailed Collaboration FRAUNHOFER

Institution	Collaboration Project	Collab. Partner	Related WP/Task	Time Frame
RWTH	SFB TRR40	TU Braunschweig, UniBw Munich	WP4, T4.3	Jul 2019 – Jun 2020
	Description: Apply dynamic mode decomposition of experimental and numerical data provided by TU Braunschweig and UniBw Munich to analyse the unsteady dynamics in the base flow field of space launchers.			
	ENODISE	VKI, TU DELFT	T4.3	June 2020 - May 2023
	Description: Apply DMD to simulation results for the analysis of acoustic ources in turbulent flow around porous material.			
	INVENTOR	ONERA, VKI	T4.3	June 2020 - May 2023
	Description: Use DMD to identify acoustic source mechanisms for landing gear noise			
	POP COE		WP2, WP3	2020
	Description: Evaluation of the performance of ZFS code using POP methods and tools. Identify bottlenecks and potential improvements.			

Table 21: Detailed Collaboration RWTH

Institution	Collaboration Project	Collab. Partner	Related WP/Task	Time Frame
TERATEC	FocusCoE,	CEA, KTH, HLRS, BSC, UCL, ENEA, PRACE, ICHEC	WP3, WP5	Dec 2019 – Nov. 2021
	Description: Coordination and implementation of activities supporting the CoEs in connecting to the industrial ecosystem in helping in promoting their services to potential clients			
	POP CoE	BSC, USTUTT, IT4I, FZ Juelich, NAG, RWTH, UVSQ	WP2, WP3	Dec 2019 – Nov. 2021
	Description: Business Development and Sustainability, assessment of the experiments and customer advocacy			

Table 22: Detailed Collaboration TERATEC

Institution	Collaboration Project	Collab. Partner	Related WP/Task	Time Frame

SSC	HLRS pilot project	HLRS Stuttgart, Federal Institute for Population Research	WP3, WP4	July 2020 -
	Description: Testing the SSC platform and its feasibility with different pilot partners and incorporating user feedback into the platform. This collaboration deals with calculations from the health care sector.			
	hydrograv GmbH	hydrograv GmbH	WP3, WP4	October 2020 -
	Description: Testing the SSC platform and its feasibility with different pilot partners and incorporating user feedback into the platform. This collaboration deals with flow simulations for the optimization of wastewater treatment plant components.			

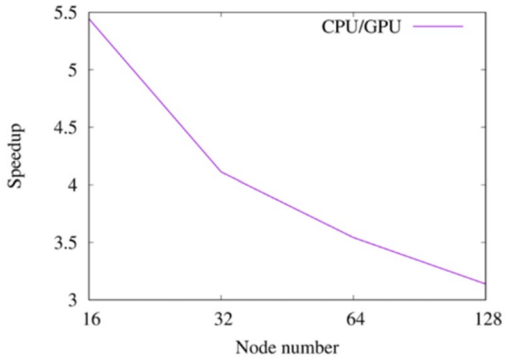
Table 23: Detailed Collaboration SSC

Annex 4: Public Collaboration Success Story: Enabling Nek5000 on GPU systems

Success Story: Enabling Nek5000 on GPU systems

SUCCESS STORY # HIGHLIGHTS:

- **Keywords:**
  - **GPU**
  - **NVIDIA**
  - **AMD**
  - **OpenACC**
  - **OpenMP**
  - **SEM**
  - **Nek5000**
- **Industry sector: Automotive, Aerospace**
- **Key codes used: Nek5000**



Speedup of the OpenACC/CUDA version for a pipe simulation performed on JUWELS Booster at JSC.

ORGANISATIONS & CODES INVOLVED:

SeRC
Swedish e-Science Research Centre

The Swedish e-Science Research Centre (SeRC) is a national e-science initiative, funded by the Swedish government Strategic Research Area Initiative, dedicated to provide e-infrastructure support and to improve important e-science software on future HPC platforms. The largest part of this support is provided by giving researchers access to the national computational experts and infrastructure and to promote collaboration between scientific experts and computational experts.

Nek5000 is an open-source code for the simulation of incompressible flows. Nek5000 is widely used in a broad range of applications, including the study of thermal hydraulics in nuclear reactor cores, the modelling of ocean currents, and the simulation of combustion in mechanical engines.

TOPIC OF COLLABORATION:

Collaboration between EXCELLERAT and SeRC is concentrated on improving the performance of the Nek5000 programme and getting Nek5000 ready to run on future hardware. There is a common interest in developing this CFD solver as it is the reference code for both EXCELLERAT and SESSI, which is one of the SeRC's research communities. This scientific code allows to perform high-fidelity simulations of relatively complex and industrially relevant flows. It shows as well very good parallel scaling properties making it a good candidate for Exascale computing.

In particular, it was necessary to port and optimise Nek5000 on GPU systems, specifically systems using hardware provided by NVIDIA and AMD. As part of the collaboration, it was necessary to examine the best practices in porting the code to the different software environments provided by AMD and NVIDIA and look at ways to re-use and standardise the work required due to the different hardware and software.

RESULTS OF COLLABORATION:

The first achievement of the collaboration between EXCELLERAT and SeRC was the extension of the CPU version of Nek5000 to run on NVIDIA GPUs using OpenACC directives. The results showing the performance of the two versions are given in Fig. 1.

After profiling the OpenACC version it was found that the directive approach was creating some inefficient small kernels. After merging some kernels by rewriting them in CUDA, a significant reduction of their total runtime was achieved, for example for calculations running on A100 machines replacing 6 OpenACC kernels in a loop with a single CUDA Fortran call reduced the runtime from 800 µs to 200 µs.

Also, as part of the profiling work, several routines were found to have significant bank conflicts when certain input was used. When these were removed the duration of the affected kernels improved by around 20%.

In addition to the OpenACC version, an OpenMP version using GPU offload has been created to enable Nek5000 to run on AMD GPUs. This is necessary due to the poor support for OpenACC provided by the AMD toolchain. The OpenMP version has currently a similar performance as the OpenACC version.

WHAT DID WE MANAGE TO DO TOGETHER THAT WE COULD NOT HAVE DONE SEPARATELY?

Before the start of the collaboration, it was only possible to run Nek5000 on CPU systems. The very good parallel scaling of the CPU version allowed the problem to scale to a large number of CPU cores, but it is clear that to run on Exascale machines it would be necessary to update Nek5000 so that it could run on GPU nodes.

In addition, the OpenACC support using the AMD toolchain is poor. Similarly, the support for OpenMP with GPU offload with the NVIDIA toolchain is also poor, so it is required to create both an OpenACC version and a version using OpenMP with GPU offload, to ensure that Nek5000 can run efficiently on both AMD and NVIDIA systems.

As a result of the collaboration, we created GPU implementations using both OpenACC and OpenMP of Nek5000, ensuring that Nek5000 is ready for use on Exascale architecture. The results of a pipe simulation experiment performed on the JUWELS Booster at Jülich Supercomputing Centre (JSC), comparing OpenACC/CUDA version and CPU version (1 node has a 48 core AMD EPYC and 4 A100 GPUs) is given in Fig. 2.

PRODUCTS/SERVICES:

- Porting existing code bases, particularly legacy codebases towards Exascale computing on GPUs using CUDA, OpenACC, and OpenMP
- provide trainings and consultancy on how to migrate large legacy codes towards Exascale computing on GPUs

UNIQUE VALUE:

Nek5000 is a code written in Fortran and C providing a good example of how to migrate large legacy codes towards Exascale. With Nek5000 being a long-established code, with very good strong scaling, the experience gained in porting Nek5000 to GPUs is highly valuable in porting other legacy codes.

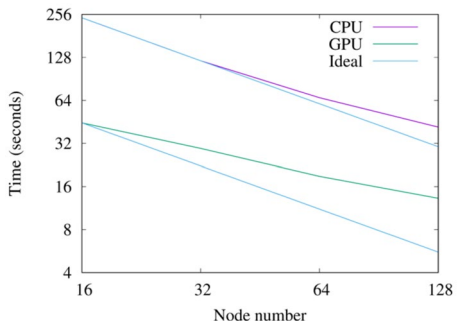


Fig. 1: Comparison of the performance of the CPU and GPU (OpenACC) version