



PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

Impact in the Digital Domain: KPIs of the High Performance Computing (HPC) infrastructure with impact on other Domains | **PRACE aisbl**

Philippe Segers

PRACE aisbl Board of Directors



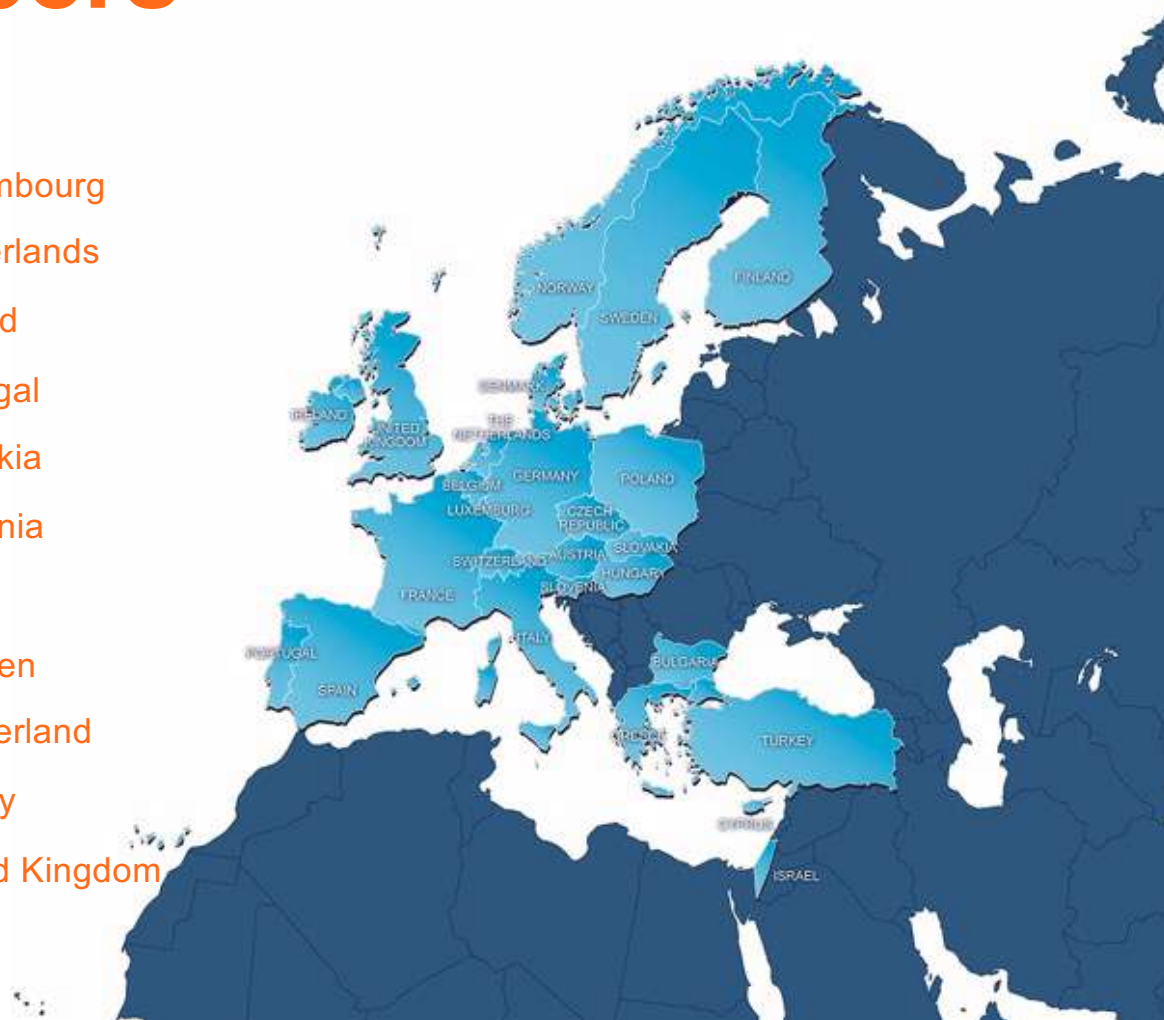
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PRACE | 27 members

- ▶ Austria
- ▶ Belgium
- ▶ Bulgaria
- ▶ Cyprus
- ▶ Czech Republic
- ▶ Denmark
- ▶ Finland
- ▶ France
- ▶ Germany
- ▶ Greece
- ▶ Hungary
- ▶ Ireland
- ▶ Israel
- ▶ Italy
- ▶ Luxembourg
- ▶ Netherlands
- ▶ Poland
- ▶ Portugal
- ▶ Slovakia
- ▶ Slovenia
- ▶ Spain
- ▶ Sweden
- ▶ Switzerland
- ▶ Turkey
- ▶ United Kingdom

Observers

- ▶ Croatia
- ▶ Romania





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PRACE | what we do

- ▶ **Open access** to world-class HPC systems to EU scientists and researchers (and world wide researchers who have cooperation in EU)
- ▶ **Variety of architectures** to support the different scientific communities
- ▶ High standards in **computational science** and engineering
- ▶ **Peer Review** at European level to foster scientific excellence
- ▶ Robust and persistent **funding scheme** for HPC supported by national governments and European Commission (EC)
- ▶ Support the development of intellectual property rights (**IPR**) in Europe by working with industry and public services
- ▶ Collaborate with European HPC **industrial** users and suppliers



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PRACE | 7 Tier-0 Systems in 2021



JUWELS Booster
Module: Atos/Bull
Sequana

GAUSS @ FZJ, Jülich,
Germany #8 Top 500



MareNostrum: Lenovo
BSC, Barcelona, Spain
#63 Top 500



Piz Daint: Cray XC50
ETH Zurich/CSCS, Lugano,
Switzerland
#15 Top 500



SuperMUC NG: Lenovo
cluster GAUSS @ LRZ,
Garching, Germany
#17 Top 500



JOLIOT CURIE: Atos/Bull Sequana
X1000; GENCI @ CEA, Bruyères-le-
Châtel, France #59 Top 500



MARCONI-100: IBM
CINECA, Bologna, Italy
#14 Top 500

NEW ENTRY 2020
HAWK: HPE Apollo
GAUSS @ HLRS,
Stuttgart, Germany
#18 Top 500



1 Petaflops is 10^{15} operations per
second (one million billion)

Close to 220 Petaflops
total peak performance
looking for Exaflops...



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PRACE 3 | 3 Basic Pillars

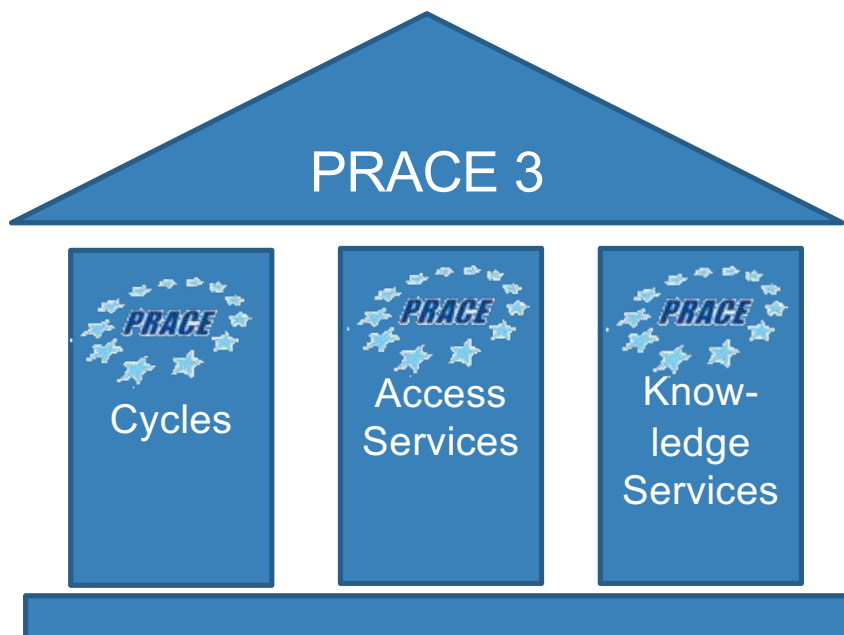
Resources

&

Services

&

People

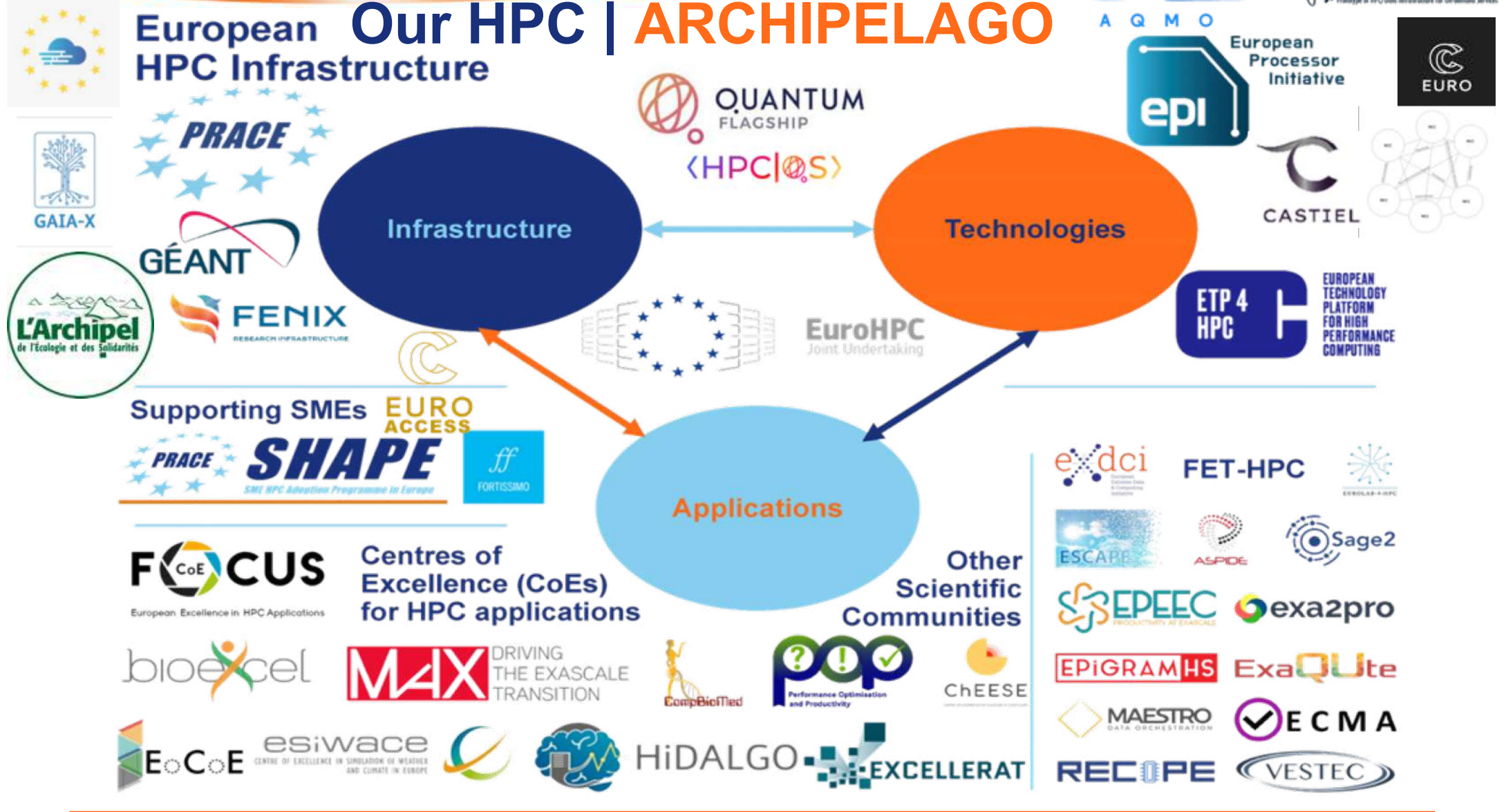


- Organisation of access calls (extreme scale, enabling, fast tracks...) for science & industry
- Peer Review process for Open Science
- Data services (Fenix, EUDAT)



- Dissemination, Communication
- Training & Education
- User Support
- Code Enabling & Development
- Technology assessment

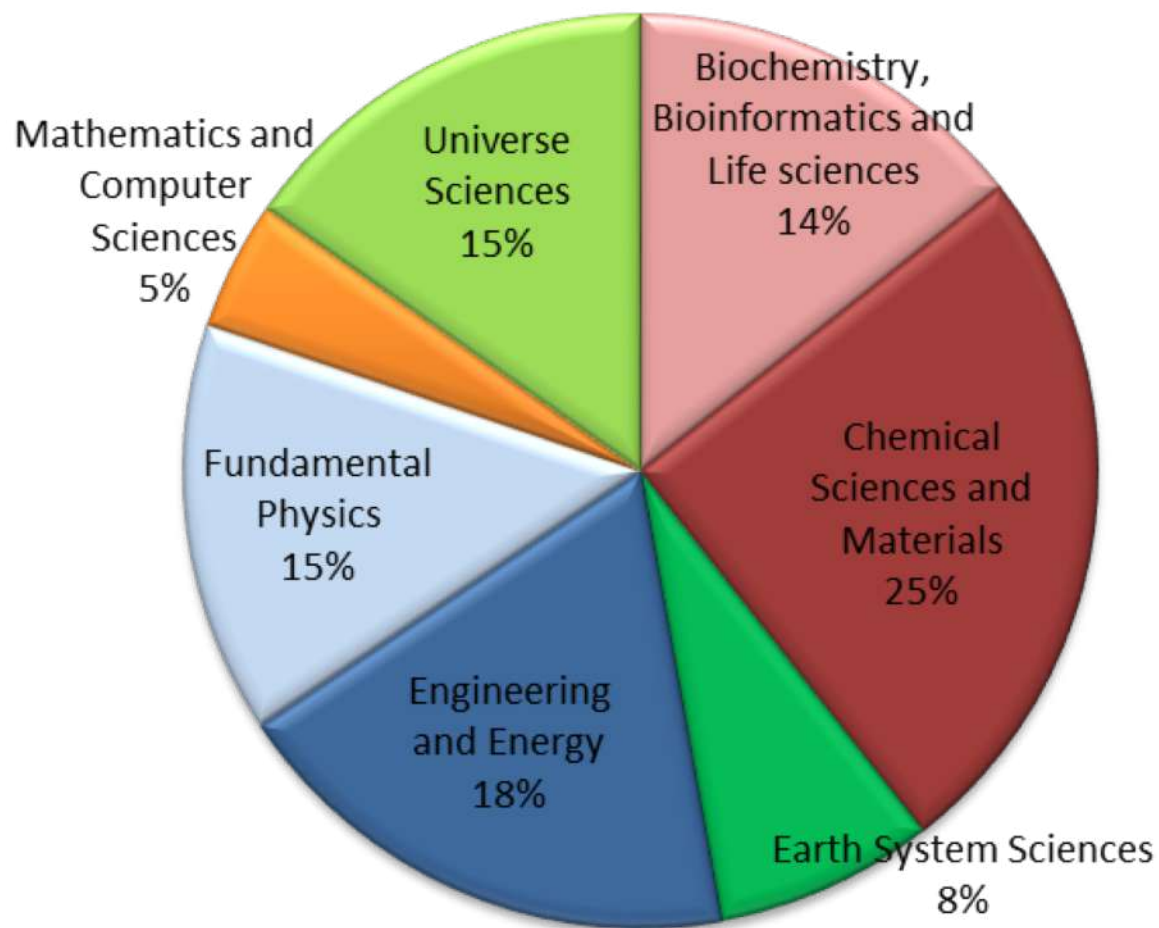






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PRACE | For all sciences





PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

PRACE | For all fields of sciences





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PRACE versus COVID-19

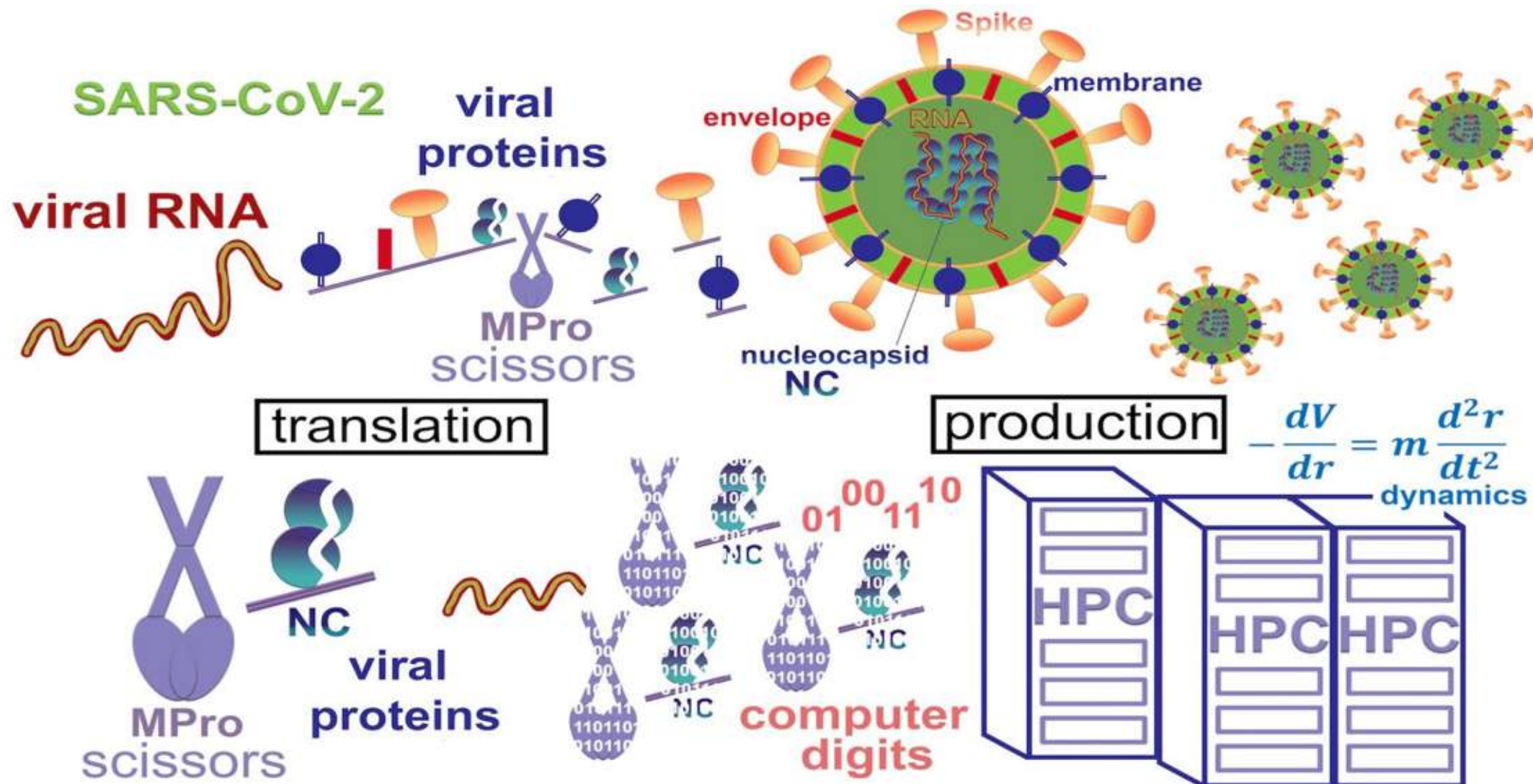
- ▶ PRACE had run a **Fast Track Call for Proposals** for projects that used supercomputers to contribute to the fight against **COVID-19. The Call closed spring 2021**
- ▶ A Scientific Committee established by PRACE had leaded the review process and evaluated proposals within **one week**
- ▶ Selected projects was given access to the **Europe's most powerful supercomputers**
- ▶ More than 30 proposals have been awarded since end of March 2020 with research topics such as:
 - ▶ Bio-simulations to develop therapeutics and/or vaccines
 - ▶ Epidemiologic analysis to understand and forecast the spread of the disease
 - ▶ Biomolecular research to understand the mechanisms of the virus infection
- ▶ PRACE Digest 2020 focusses on projects awarded under the Fast Track Call





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- ▶ Using Molecular Dynamics To Find Drugs And Vaccines For COVID-19
 - ▶ PI Vangelis Daskalakis of the Cyprus University of Technology
 - ▶ <https://prace-ri.eu/using-molecular-dynamics-to-find-drugs-and-vaccines-for-covid-19/>





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PRACE | SHAPE

Innovation & Impact

- ▶ **SME HPC Adoption Programme in Europe (SHAPE)**
 - ▶ Equip European SMEs with expertise to take advantage of the innovation possibilities of HPC and AI
 - ▶ Increasing competitiveness
 - ▶ Enable development of new products or services
 - ▶ Create new business opportunities



SHAPE
SME HPC Adoption Programme in Europe



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PRACE | scientific case

- ▶ First edition in 2012, update in 2018
- ▶ We cannot do it all
 - ▶ Which application domains to focus on?
 - ▶ Which technologies?
- ▶ Eternal struggle: heavenly Science vs mundane Economics
- ▶ Balance between traditional, disruptive and fundamental science



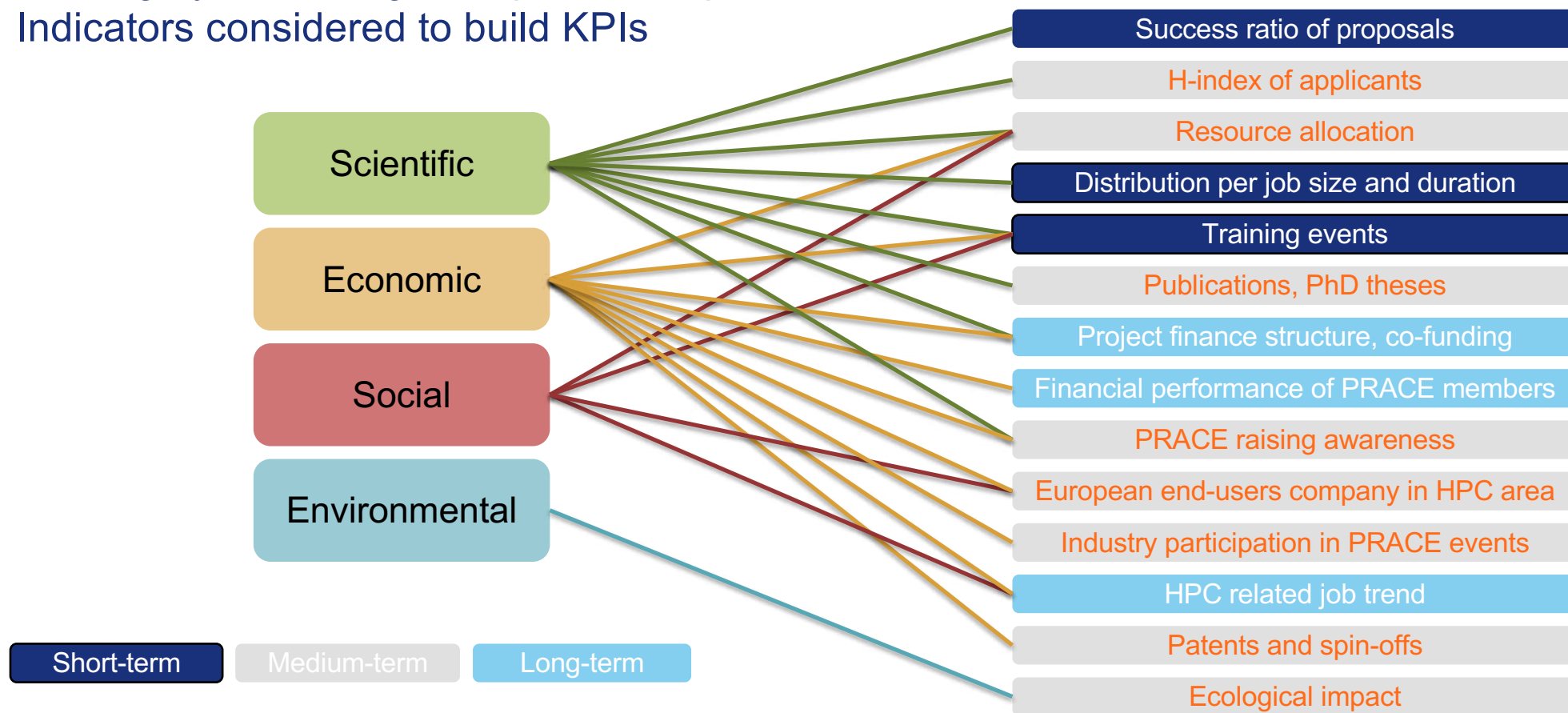


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Impact | how to assess it ?

Starting by assessing our operational performance

Indicators considered to build KPIs

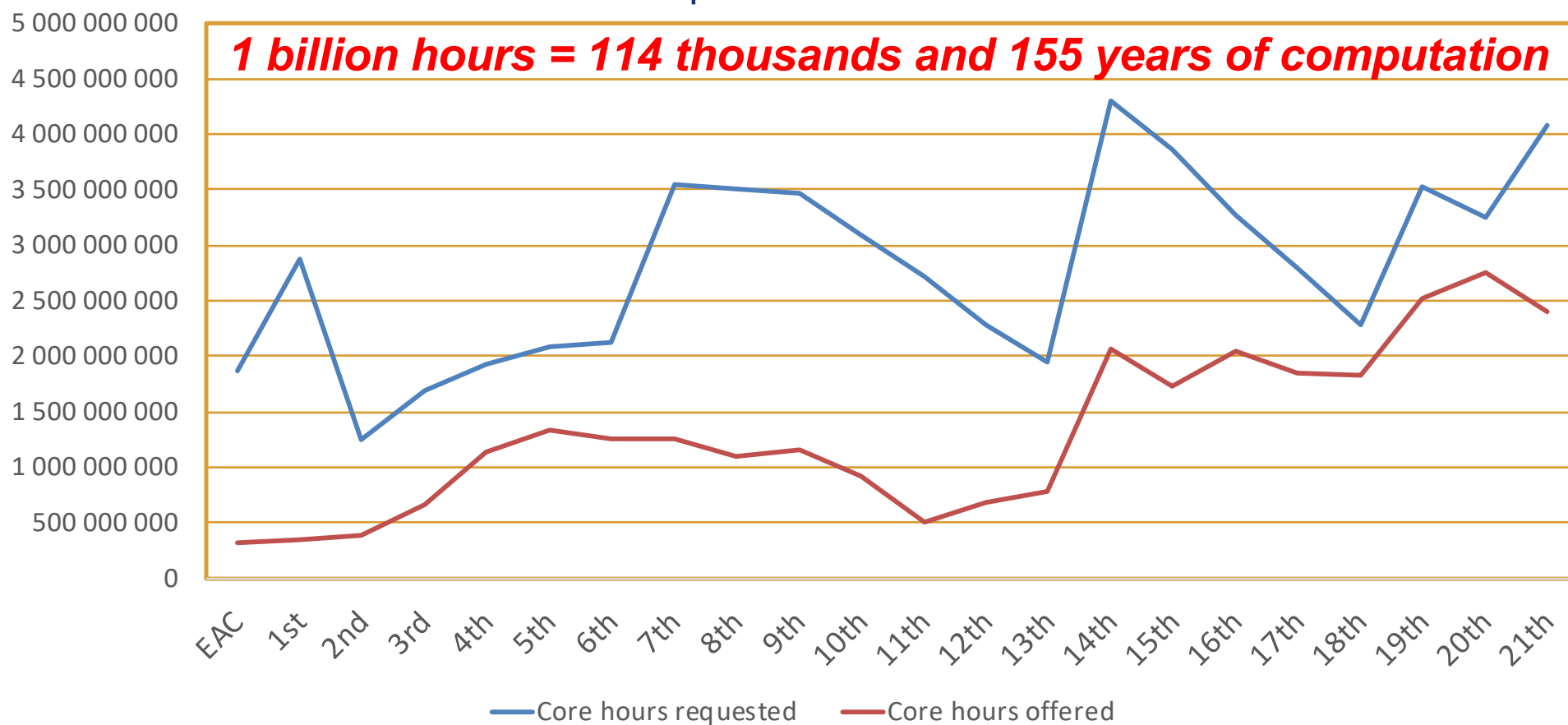




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PRACE | Project Access

Core hours offered and requested in each PRACE call

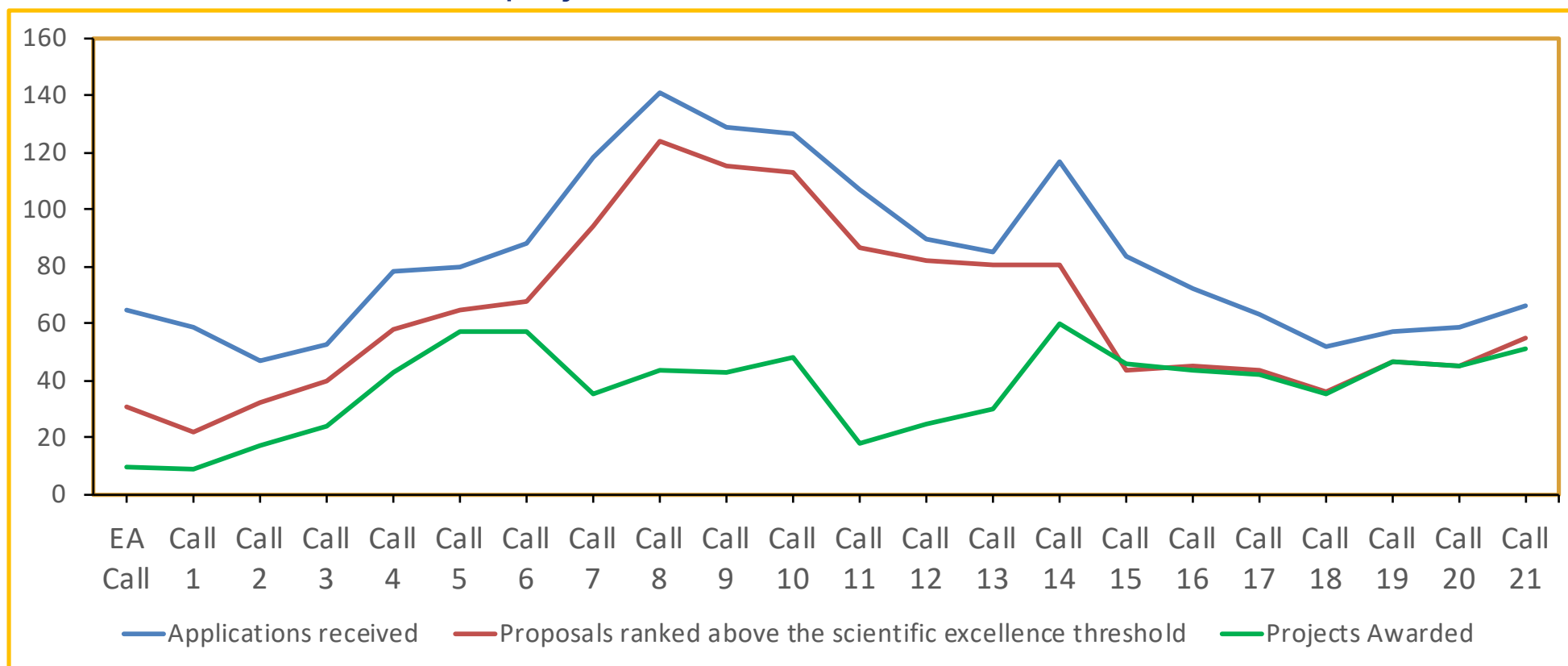




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PRACE | Projects Awarded & Rejected

Total number of applications received, proposals ranked above the scientific excellence threshold, and projects awarded

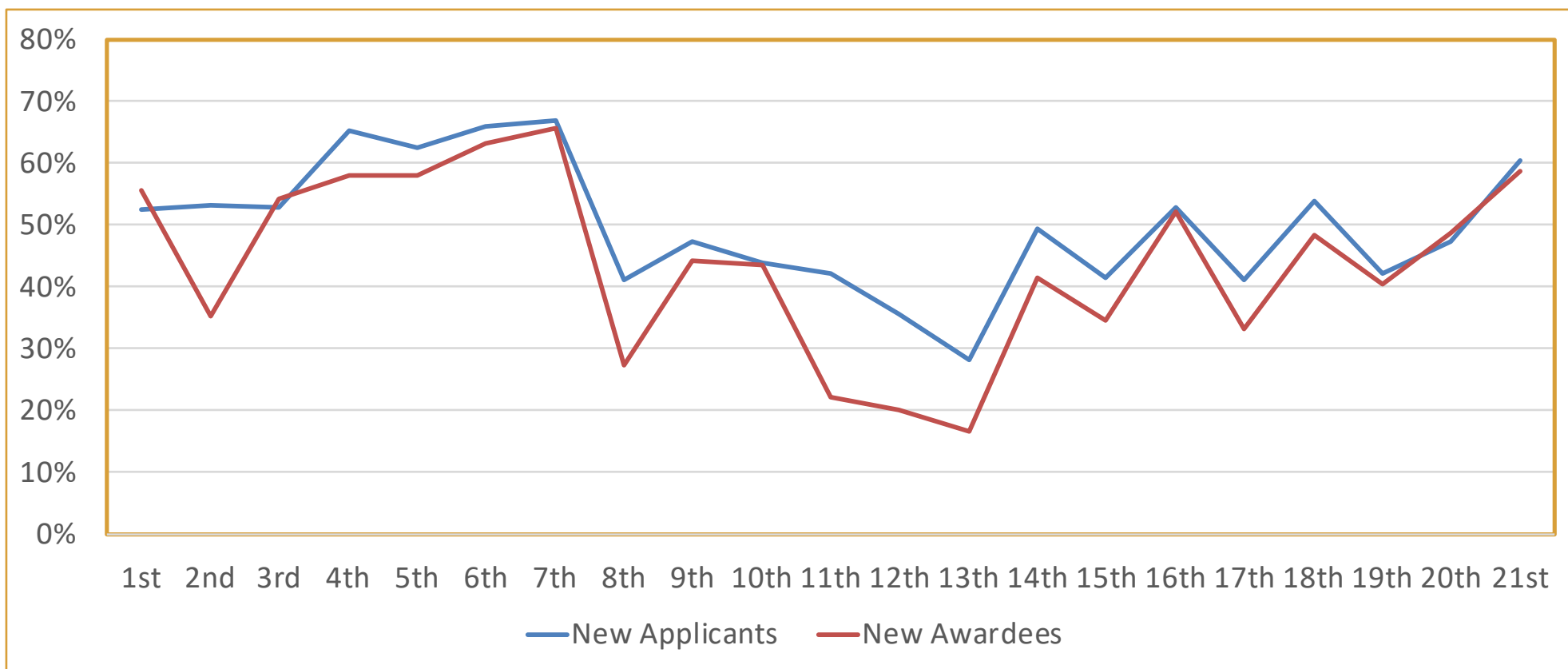




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PRACE | Recurring users

Ratio of new applicants and new awardees in each PRACE call

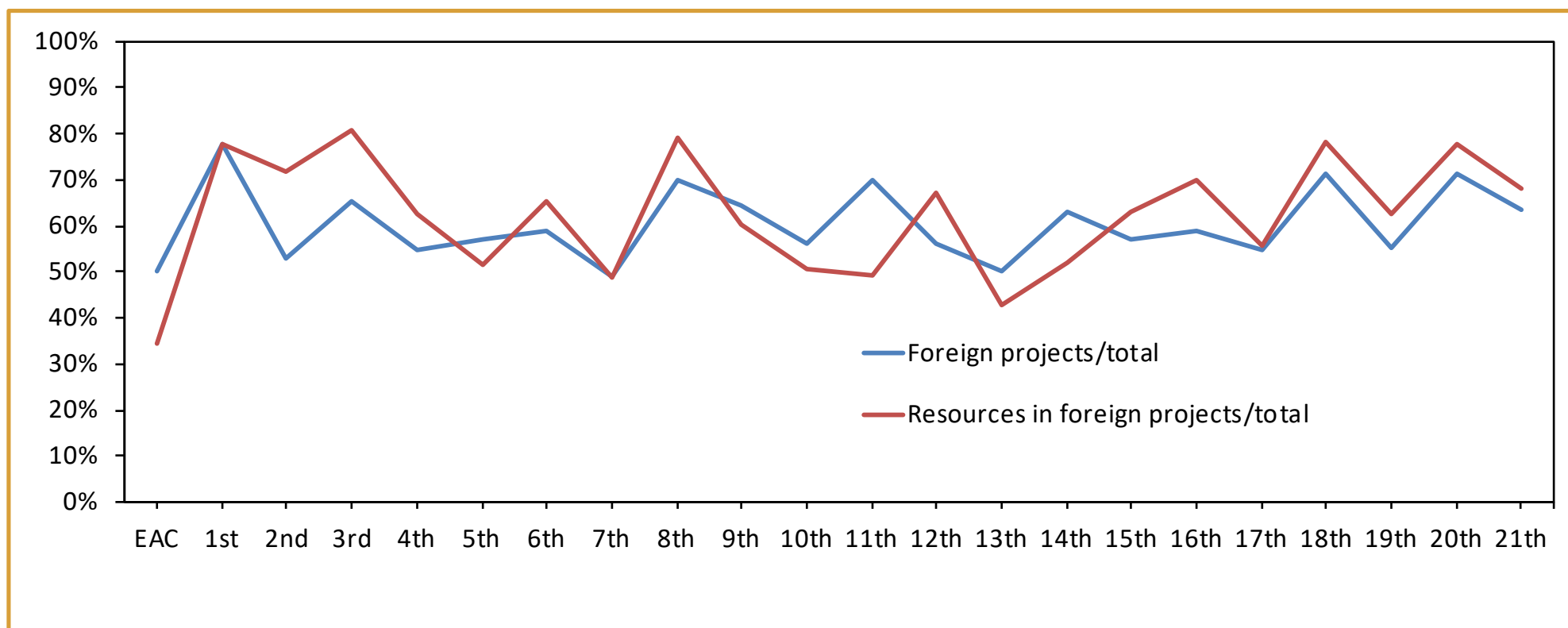




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PRACE | 'foreign' projects

Ratios of awarded 'foreign' projects and resources for awarded 'foreign' projects

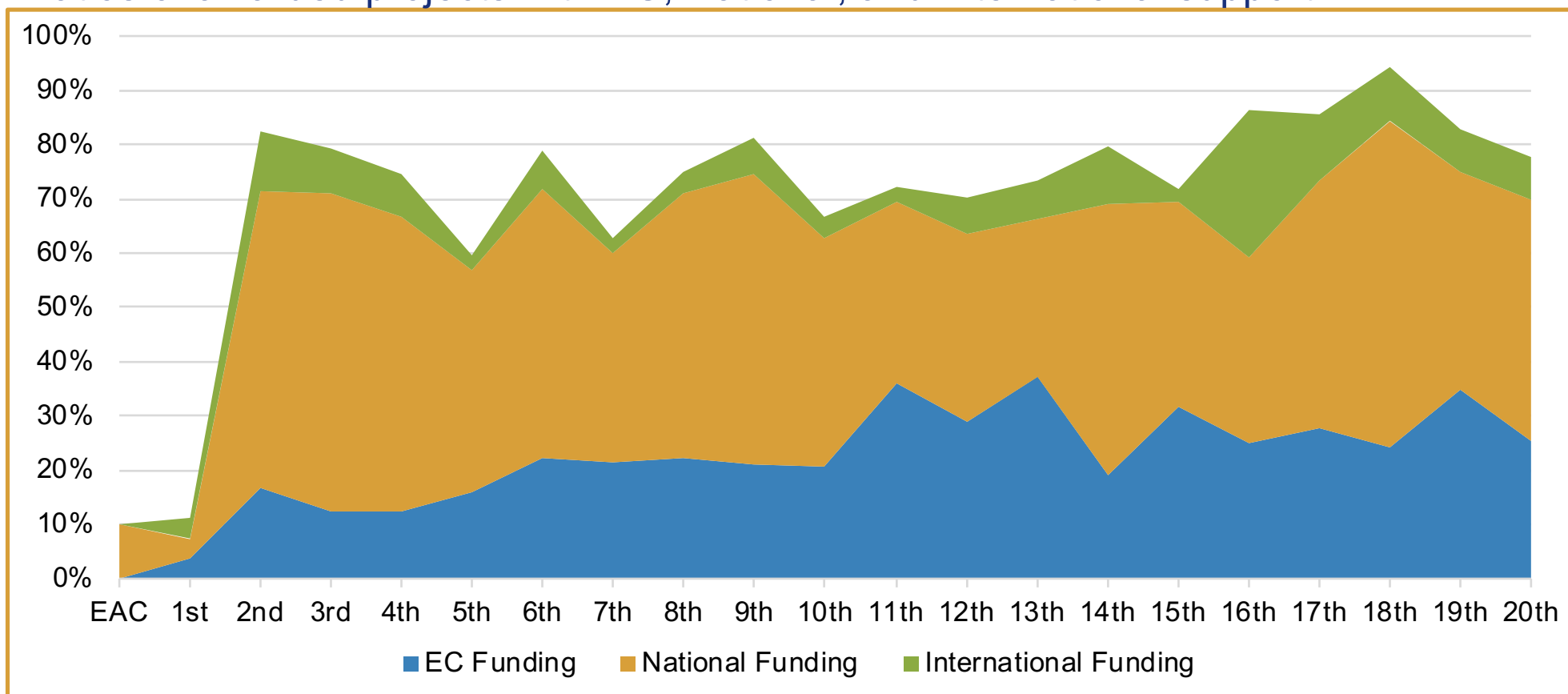




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PRACE | Co-funding

Ratios of awarded projects with EC, National, and International support

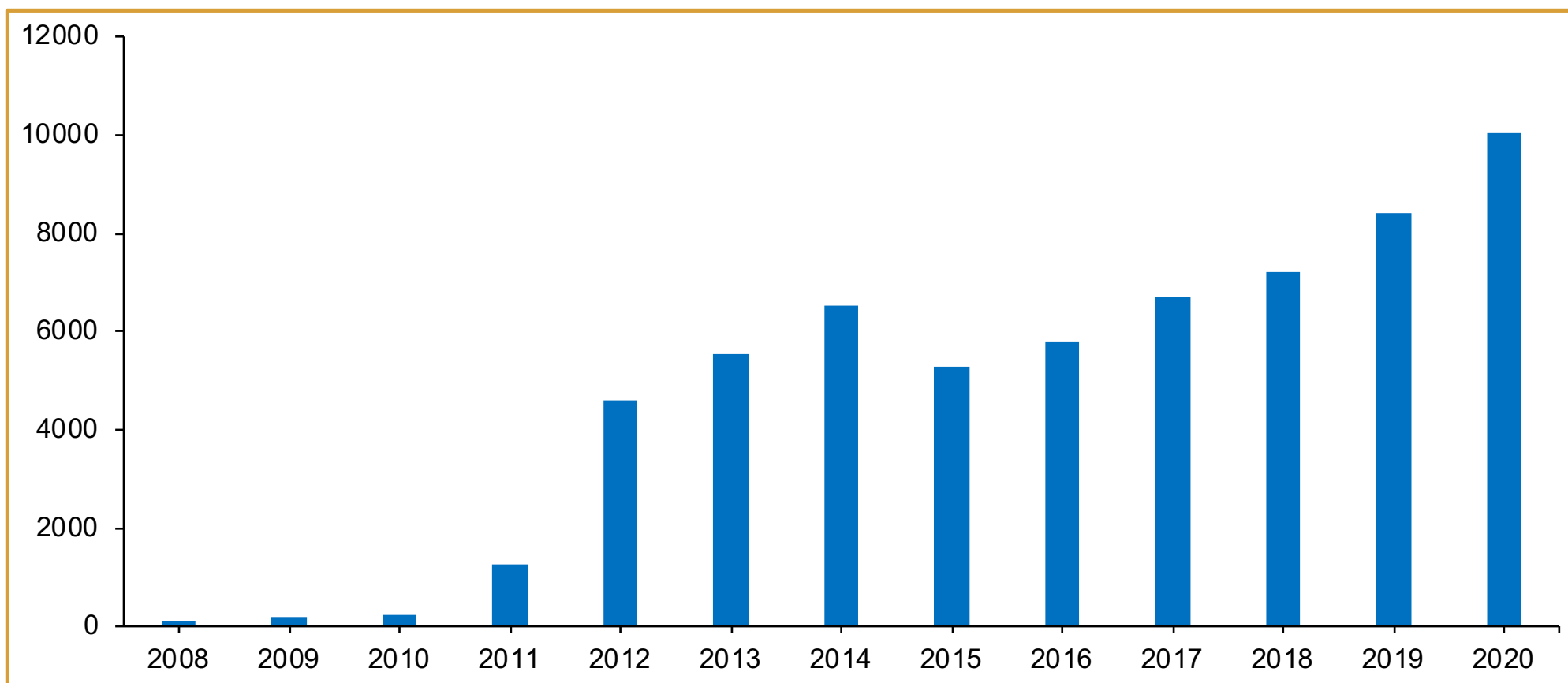




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PRACE | Training

Numbers of person-days registered at PRACE Training Centres between 2008 and 2020

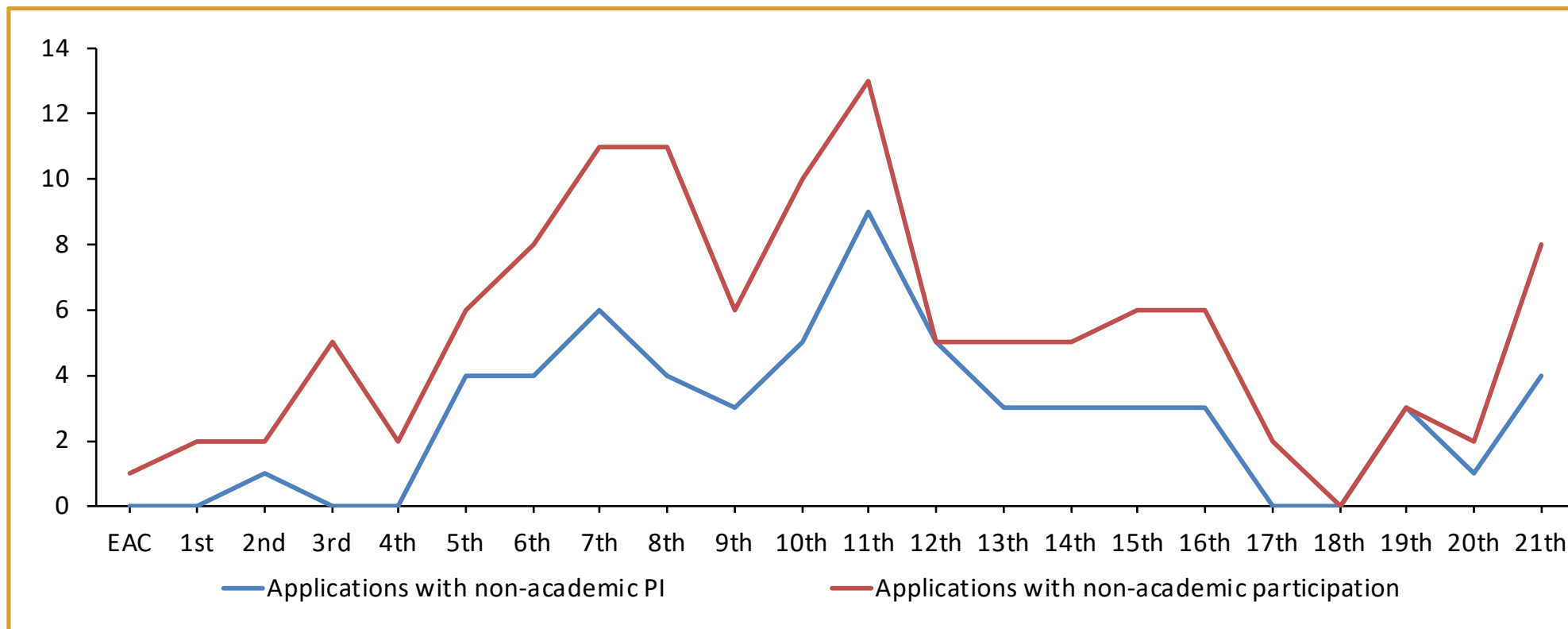




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PRACE | Industry

Industry participation in PRACE





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Data collection

- ▶ Database from the peer-review tool:
 - ▶ Compiles all information on the calls (resources awarded, machines, project participants, collaborators affiliation, industry partners, etc.)
- ▶ Surveys to projects leaders:
 - ▶ Final report at the end of the allocation period
 - ▶ Follow-up 2 years after
- ▶ Spreadsheet for training events
- ▶ Media coverage



Limitations and specificities

- ▶ Time-frame between computation and scientific/economic exploitation:
 - ▶ Need to stay informed about publications several years after the allocation is done
 - ▶ Long-term impact on competitiveness of industry?
 - ▶ Complex infrastructure:
 - ▶ Distributed
 - ▶ Virtual access
 - ▶ Shared by multiple scientific communities and type of users
 - ▶ A difficult multi-factors impact assessment:
 - ▶ Broad range of actors in the ecosystem: scientists, industrials, vendors, computing centers...
 - ▶ Qualitative (success stories, etc.) more than quantitative
 - ▶ How to assess the overall increase in HPC adoption?
 - ▶ Impact of HPC in European competitiveness embedded in the whole value chain
- Lack of consistent economic and scientific data



Limitations and specificities

► Internal limitations:

- KPIs defined after the infrastructure
- Historical data not structured to facilitate impact assessment
- Not always possible to know usage at the time of data collection
- Limited resources
- Some manual processing
- Citation are still not always provided
 - *do you acknowledge your laptop for your research?*

► Two levels of impact assessment:

- At a European level, for the PRACE infrastructure and HPC in general
- At a national level, for hosting a system or participating in the infrastructure



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Conclusion on KPI

- ▶ PRACE: a distributed e-Infrastructure devoted to serve its users
- ▶ PRACE Key Performance Indicators:
 - ▶ A tool for continuous improvement process
 - ▶ Designed to assess the fulfilment of its mission
 - ▶ Covering a wide spread of interactions with its stakeholders
- ▶ But KPI is **not** a direct measurement of impact of our IR...



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PRACE | achievements / impacts

- ▶ 873 scientific projects enabled
- ▶ >30 billion core hours awarded since 2010 (3.4 million years of computation)
- ▶ Of which 63% led by another PI nationality than the HM
- ▶ R&D access to industrial users with >65 companies supported
- ▶ >17 000 people trained through PRACE Training
- ▶ ~220 Petaflops of total peak performance on 7 world-class systems
- ▶ 27 PRACE members, including 5 Hosting Members (France, Germany, Italy, Spain and Switzerland)
- ▶ PRACE is the only e-infrastructure Landmark on the ESFRI Roadmap 2016



PRACE | impact

- ▶ **Scientific Impact** = compute power x operation efficiency x allocation efficiency x code efficiency x knowledge of the RI x knowledge of HPC x quality of the research x number of (European) PI & researchers
- ▶ Taken that Compute systems change every 5 years
 - ▶ Which application domains to focus on?
 - ▶ Which technologies?
- ▶ **Innovation impact** = Scientific Impact x innovation conversion factor
- ▶ **Job impact** = Innovation impact x intensity of manpower needed
- ▶ **Impact on society?** We know better that Climate Change is coming...
- ▶ Trade-off to be considered
 - ▶ Higher computation performance means higher “cost of coding”
 - ▶ How to balance long term training and fast technology changes?



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THANK YOU FOR YOUR ATTENTION

www.prace-ri.eu



EuroHPC
Joint Undertaking

**EuroHPC
Summit Week 2022**



#PRACEdays

EuroHPC Summit week 2022 Goes to Paris

► You are all welcome !



From 21 to 24 March 2022, first HPC live event since ??? **#EHPCSW**