



arnes 



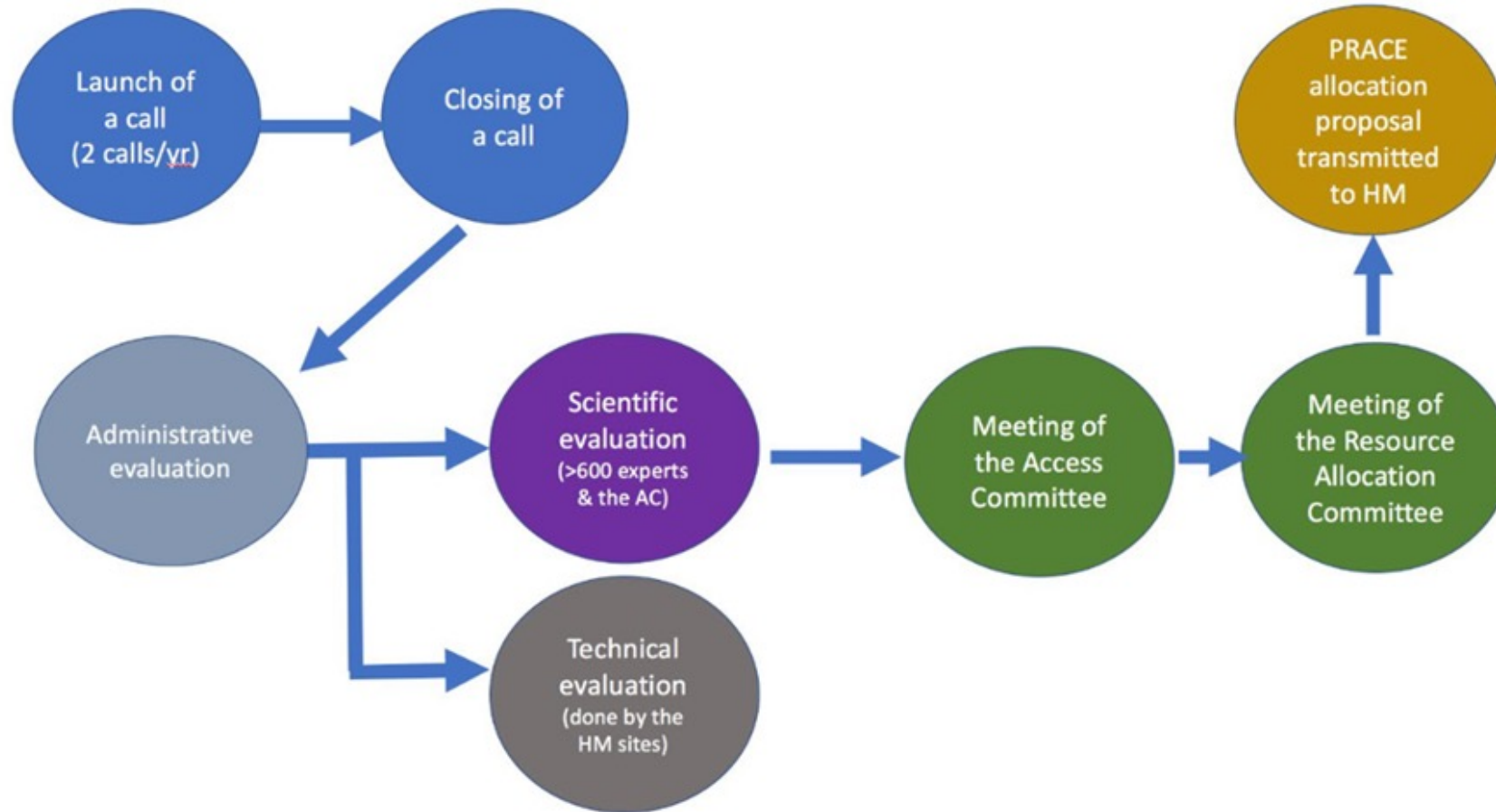
NIxOS
National Initiatives for Open Science in Europe

**Urgentno superračunalništvo v boju proti
pandemiji**

Matej Praprotnik, Kemijski inštitut in UL FMF
Mreža znanja 2021, od 23. do 30. novembra

Pravila odprtega dostopa (povzeto po PRACE)

Review process overview & administrative assessment



Povzetek pravil odprtega dostopa

- **KOMISIJA ZA DOSTOP:** predsednik, podpredsednik, panel ekspertov (znanstvene discipline)
- **TIPI DOSTOPOV:** nacionalni odprti dostop SLING (1), namenska lastniška uporaba (2), souporaba po dogovoru (3)
- **ALOKACIJA VIROV:** računske (1), diskovne (2), omrežne (3) kapacitete in zahteve po ekspertni pomoči uporabnikom (4)
- **UPRAVIČENOST:** vsi, ki imajo dostop do omrežja Arnes (1), industrijski raziskovalni centri (2), tuji raziskovalci vpleteni v domače projekte (3), s strani domačih entitet potrjeni veliki mednarodni znanstveni in raziskovalni centri (4)
- **TIPI PROJEKTOV:**
 - Razred A: Zelo veliki projekti tipa PRACE (velikostni razred do 10 mio jeder ur)
 - Razred B: Običajni projekti (recimo do 1,5 mio jeder ur)
 - Razred C: Razvojni projekti za raziskave in testiranje (100 k jeder ur)
 - Razred D: Projekti za merjenje zmogljivosti, testiranje, razvoj in skaliranje (10 k)
- **POROČILA IN PONOVI DOSTOPI:**
 - Poročila glede na tip projekta, možna obnova

Vsi dosedanji uporabniki bodo uvrščeni v tipe projektov razreda D ali C.

PRACE Covid-19 Fast Track Call





PRACE support to mitigate impact of COVID-19 pandemic

Fast Track Call for Proposals

1 Scope

PRACE is welcoming project proposals requesting computing resources to contribute to the mitigation of the impact of the COVID-19 pandemic. This applies, without being exhaustive, to the following topics:

- Biomolecular research to understand the mechanisms of the virus infection
- Bioinformatics research to understand mutations, evolution, etc.
- Bio-simulations to develop therapeutics and/or vaccines
- Epidemiologic analysis to understand and forecast the spread of the disease
- Other analyses to understand and mitigate the impact of the pandemic

This call for proposals will follow a fast track review process to provide swift feedback to the applicants.

This call is open until further notice. Applications are evaluated within one week and start as soon as possible if awarded.

2 Who can apply and what can you apply for?

Researchers from academia, from research institutes, and from commercial organisations (industry) based in Europe are eligible to apply.

Awardees in this call commit to publish the outcome of their project as preprint and as soon as possible, to make the data available following open data policy, and to acknowledge the use of the corresponding resources and the PRACE RI.

They can apply for resources offered by PRACE on the following systems:

- Joliot-Curie, Bull Sequana X1000 / XH2000, GENCI@CEA, France
<http://www-hpc.cea.fr/en/complexe/tgcc-JoliotCurie.htm>
- HAWK, HPE Apollo, GCS@HLRS, Germany
<https://www.hlrs.de/systems/hpe-apollo-hawk/>
- JUWELS, BULL Sequana X1000 / XH2000, GCS@JSC, Germany
https://www.fz-juelich.de/fas/jsc/EN/Expertise/Supercomputers/JUWELS/JUWELS_node.html
- SuperMUC-NG, Lenovo ThinkSystem, GCS@LRZ, Germany
<https://doku.lrz.de/display/PUBLIC/SuperMUC-NG>
- Marconi 100, IBM Power 9 AC922 Whisperspoon, CINECA, Italy
<https://wiki.u-gov.it/confluence/display/SCAIUS/UG3.0%3A+System+Specific+Guides>
- MareNostrum 4, Lenovo System, BSC, Spain
<https://www.bsc.es/marenostrum/marenostrum/technical-information>
<https://www.bsc.es/user-support/mn4.php>
- Piz Daint, Cray XC50 System, ETH Zurich / CSCS, Switzerland
<https://www.cscs.ch/computers/piz-daint>
<https://user.cscs.ch/>



Applicants may also consider resources made available through the PRACE-ICEI call <https://prace-ri.eu/hpc-access/collaborative-calls/prace-icei-calls-for-proposals/#AvailableResources>

We estimate that projects with a duration of three to six months and sized from 30 million to 50 million core hours will address the topics appropriately. Nevertheless, this does not preclude projects with other sizes and duration to be awarded.

Applicants may also identify specific additional resource requirements to successfully complete their project, for instance support to adapt their tool chain to the computing and data infrastructure, see e.g. <https://prace-ri.eu/training-support/>.

3 Proposal requirements and how to apply

The following elements are expected to be provided by the applicants to describe their proposal:

- Short description of the scientific goals and objectives (1 page)
- Required resources (1/2 page)
- Description of the research methods, algorithms, and tool chain (1/2 page)
- Description of special needs (if any)

To submit proposals, fill out the application form available at

https://prace-ri.eu/wp-content/uploads/PRACE_COVID-19_ApplicationForm-v5.docx

and send it by email to covid-19@prace-ri.eu.

4 Review process and criteria

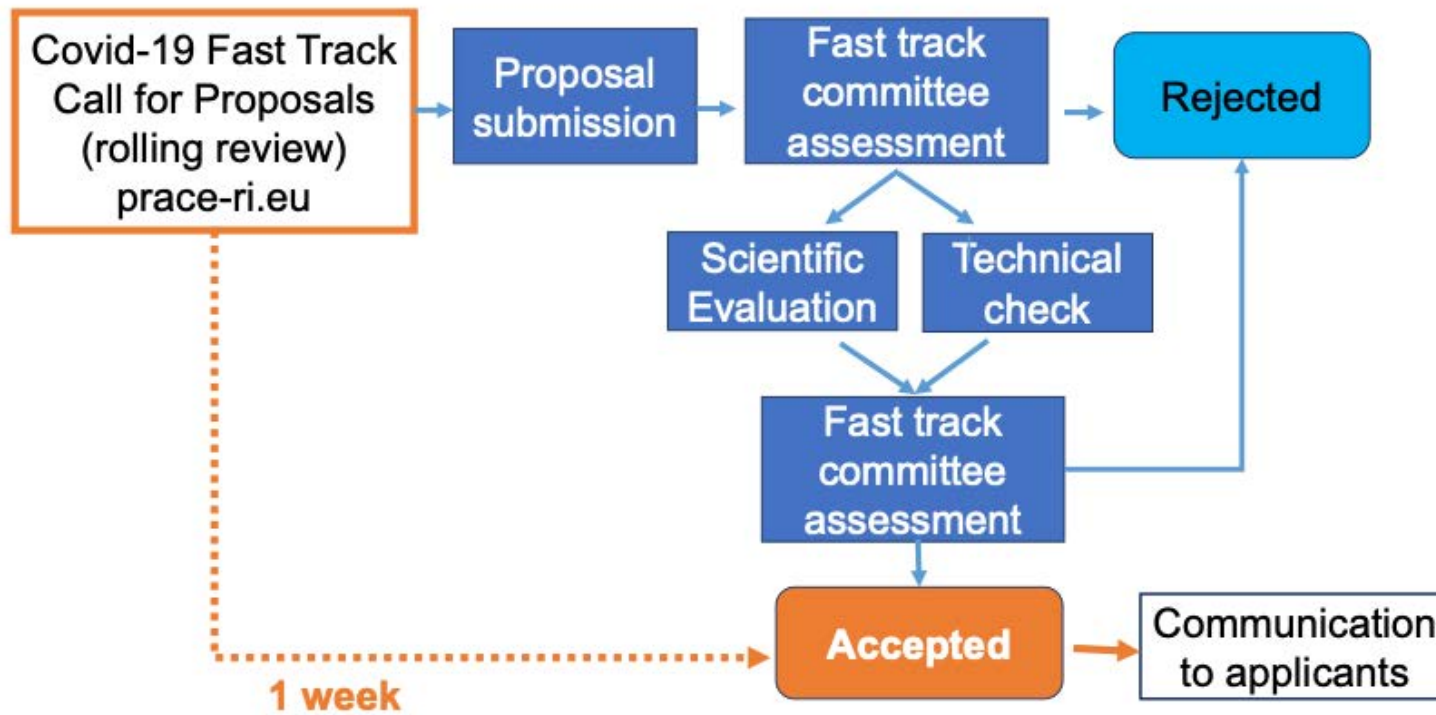
A Scientific Committee will be established by PRACE and composed of members of the PRACE Access Committee (AC) and PRACE Scientific Steering Committee (SSC) – which are groups of leading international scientists and engineers. They will discuss the merit of the proposals, supported by external scientific experts, and a technical team, based on the criteria listed below.

Significance of the Proposal: Is the proposal addressing the scope of the call? Is the expected impact aligned with the objective of the call?

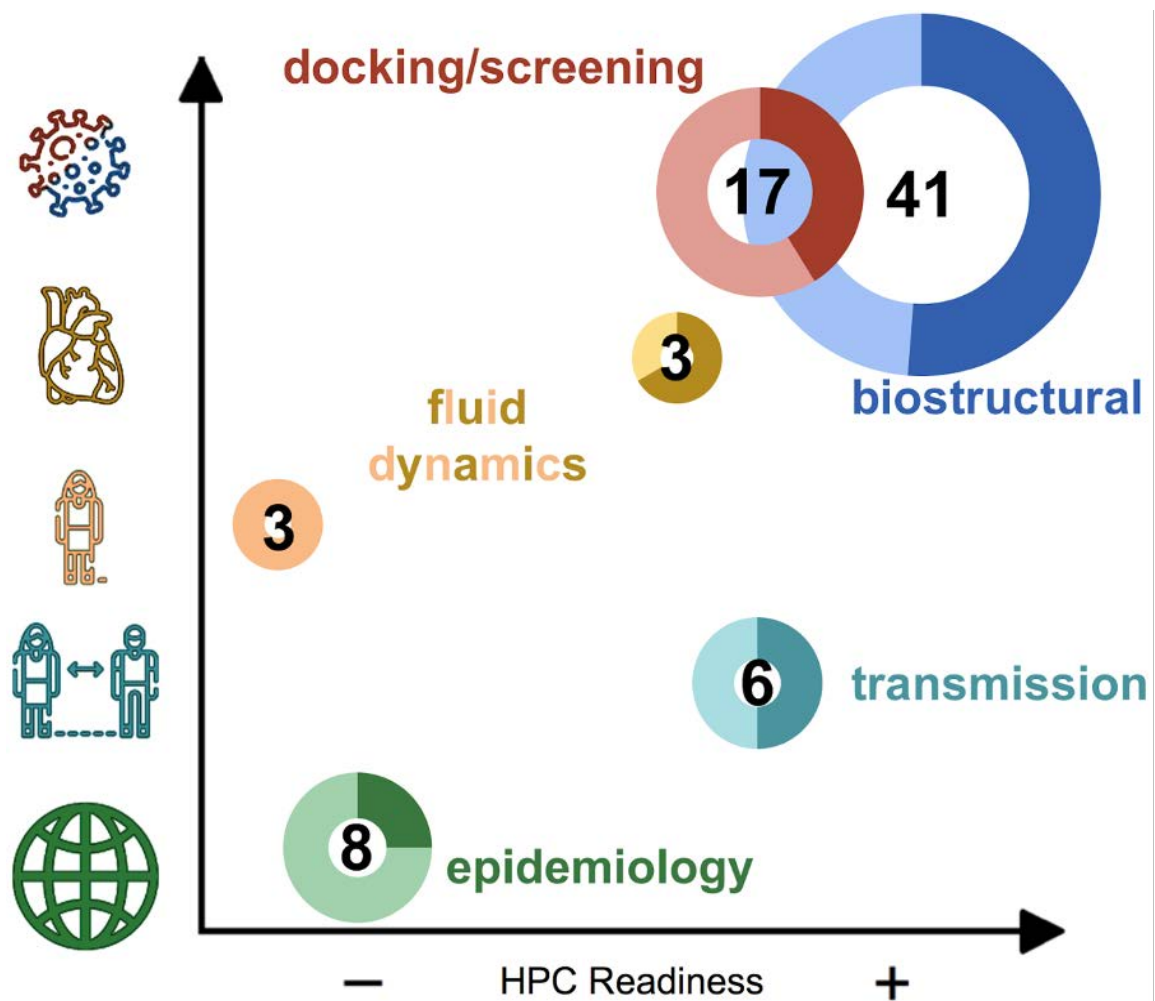
Soundness of the Methodology and Tools: Does the request describe appropriate tools, methods, and approaches for addressing the objectives?

Technical Feasibility: Are the codes and tools already available and tested on the target systems or is there a reasonable plan to achieve that quickly?

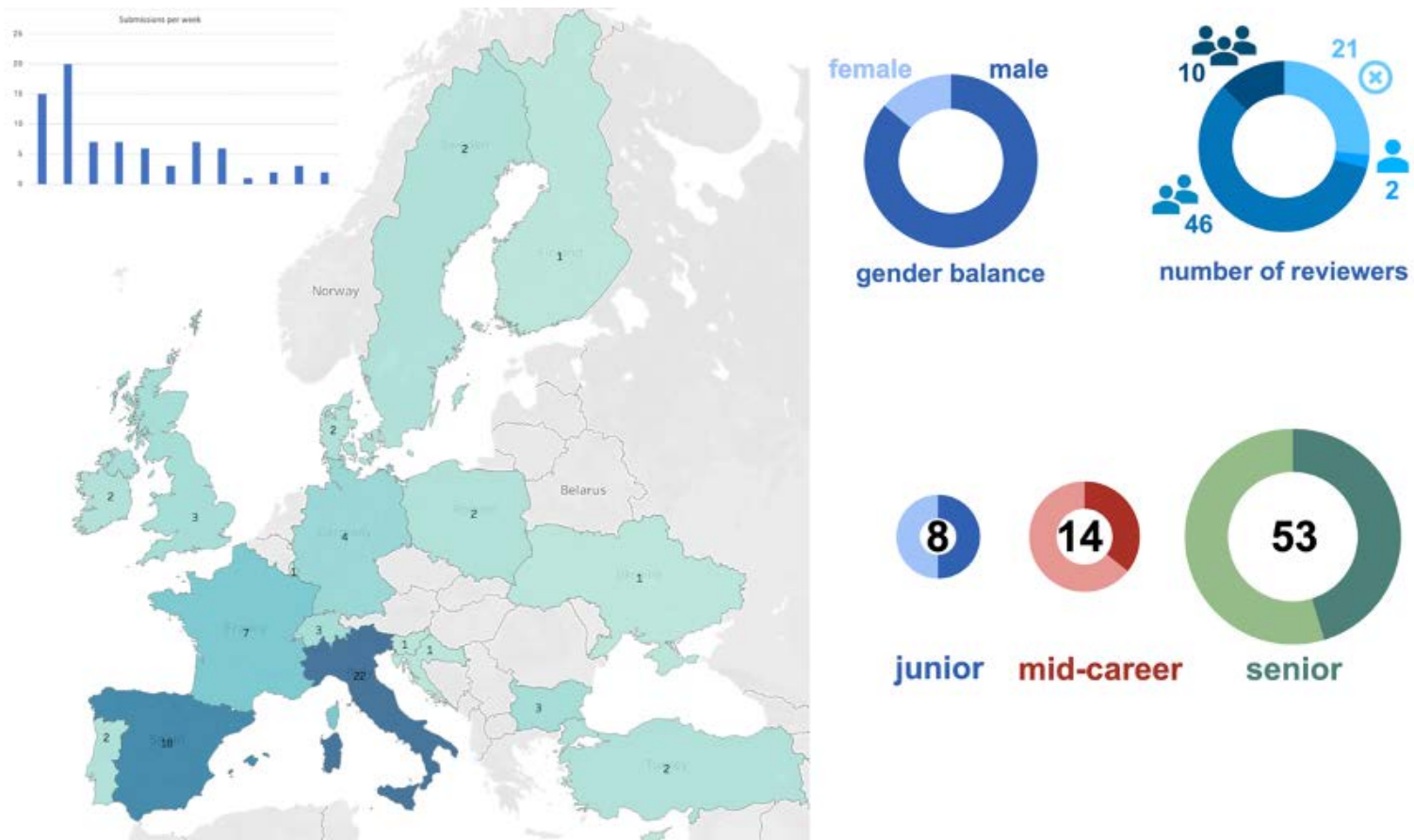
Shema procedure za prijavo na PRACE Covid-19 Fast Track Call



Pregled prijavljenih projektov



Statistični pregled prijav po državah





Foreword



Fighting the pandemic with HPC

This edition of the PRACE Digest focusses entirely on projects awarded under the PRACE Fast Track Call for Proposals to mitigate the impact of the COVID-19 pandemic.

PRACE opened this Call for Proposals in early spring as an urgent computing answer to the need for fast scientific discovery to find ways to stop the spread of SARS-CoV-2, reduce its impact on our health and economy, and find treatments for people affected by the disease.

A Scientific Committee of five high-level researchers has been leading the review process and evaluating proposals within one week. Selected projects are given access to the Europe's most powerful supercomputers. Those projects can also receive data storage and sharing solutions, e.g. from FENIX and ICEI, in line with the open data policy applicable to the Call.

Over 80 project applications have been received and, with an acceptance rate of less than 50%, just over 30 projects have been awarded time on one of PRACE's world-class systems. In total, half a billion computational hours have been awarded over a period of six months.

The pandemic has brought researchers together like never before, encouraging collaboration across all disciplines in order to find answers in a time when we need them most. Projects awarded under the Fast Track Call come from fields such as biomolecular simulations, bioinformatics, epidemiology, computational fluid dynamics, screening and docking, among others. Furthermore, monthly webinars have been organised with our colleagues in the USA, where project leaders from around the world have presented their work and exchanged on solutions and collaborations concerning the pandemic research.

I highly encourage you take inspiration from the articles in this edition of the PRACE Digest to develop further innovations to tackle the coronavirus pandemic.

Please also save the dates of the next edition of the *EuroHPC Summit Week*, which will be held digitally from 22 to 26 March 2021, and which will include an entire day of talks and presentations of COVID-19 related research.

Matej Praprotnik

*Head of the Laboratory for Molecular Modeling at the
National Institute of Chemistry, Ljubljana, Slovenia
Professor of Physics at the University of Ljubljana, Slovenia
Chair of the PRACE Scientific Steering Committee
Member of the Scientific Committee for the PRACE Fast Track Call
for Proposals to mitigate the impact of the COVID-19 pandemic*

Zahvala
PRACE, PRACE SSC, PRACE AC

