BENCHMARK ACCESS CALL & DEVELOPMENT ACCESS CALL ve ÇAĞRILARA İLİŞKİN DOKÜMANLAR

Merve DEMİRTAŞ
TÜBİTAK ULAKBİM

BENCHMARK ACCESS CALL

- Kullanılacak kodların/uygulamaların hedef sistemlerdeki performans verilerinin toplanması için başvurulur.
- Kodlar için gerekli parametler optimize edilir ve probleme uygun kaynak ihtiyacı belirlenir.
- Erişim süresi 2-3 aydır.
- Bu çağrı ile mevcut kaynakların sadece çok küçük bir yüzdesi tahsil edilir.
- Akademisyenler, kamu yetkilileri ve endüstri temsilcileri başvuru yapabilir.

Başvuru Tarihleri

- 1 January 2022 – 11:00 AM CET
- 1 February 2022 – 11:00 AM CET
- 1 March 2022 – 11:00 AM CET
- 1 April 2022 – 11:00 AM CEST
- 1 May 2022 – 11:00 AM CEST
- 1 June 2022 – 11:00 AM CEST
- 1 July 2022 – 11:00 AM CEST
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- 1 October 2022 – 11:00 AM CEST
- 1 November 2022 – 11:00 AM CET
- 1 December 2022 – 11:00 AM CET

Değerlendirme Süreci ve Kriterler

- Çağrı sürekli açıktır.

- Değerlendirme süreci maksimum 2 hafta içinde gerçekleşir.

- Bu süreçte bir bilimsel değerlendirme olmamaktadır:
    >>> İdari kontrol
    >>> Talep ile hedeflenenin uygun olması: Kaynak tahsis edilen kurumun uzmanları tarafından değerlendirme.

Sürecin Tamamlanması

- Başvuru sahiplerinden karşılaşılaşılan zorluklar, uygulanan çözümler, erişimin sonucu hakkında kısa bir rapor yazmaları beklenmektedir.

- Diğer çağrılara başvuru yapılması durumunda (Regular Access v.b.) Benchmark kapsamında elde edilen sonuçlar kullanılır.

DEVELOPMENT ACCESS CALL

- Kod ve algoritma geliştirmeye odaklanan optimizasyon projeleri için tasarlanmıştır.
- Akademi, kamu ve özel sektör temsilcileri başvuru yapabilir.
- Kod ya da algoritmanın ihtiyacına yönelik sınırlı kaynak tanımlanır.
- Çağrı sürekli açıktır.
- Erişim süresi 1 yıla kadar uzatılabilir ve 2 defa da yenilenebilir.
- Center of Excellence gibi mükemmelliyet merkezlerini ya da NCC 'leri çalışmalarını destekleyecek projeler için özel uygulamalar mevcuttur.

Değerlendirme Süreci ve Kriterler

- Değerlendirme süreci maksimum 2 hafta içinde gerçekleşir.
- Bu süreçte bir bilimsel değerlendirme olmamaktadır:

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DEVELOPMENT ACCESS CALL

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Sürecin Tamamlanması

❑ Başvuru sahiplerinden projelerinin sonuçları hakkında bir rapor hazırlaması beklenmektedir.

❑ Hazırlanan raporda:

- Hedeflere ulaşılması.
- Karşılaşılan teknik sorunlar ve nasıl aşıldığı.
- Altyapı ile ilgili karşılaşılan problemler.

BENCHMARK ACCESS CALL & DEVELOPMENT ACCESS CALL

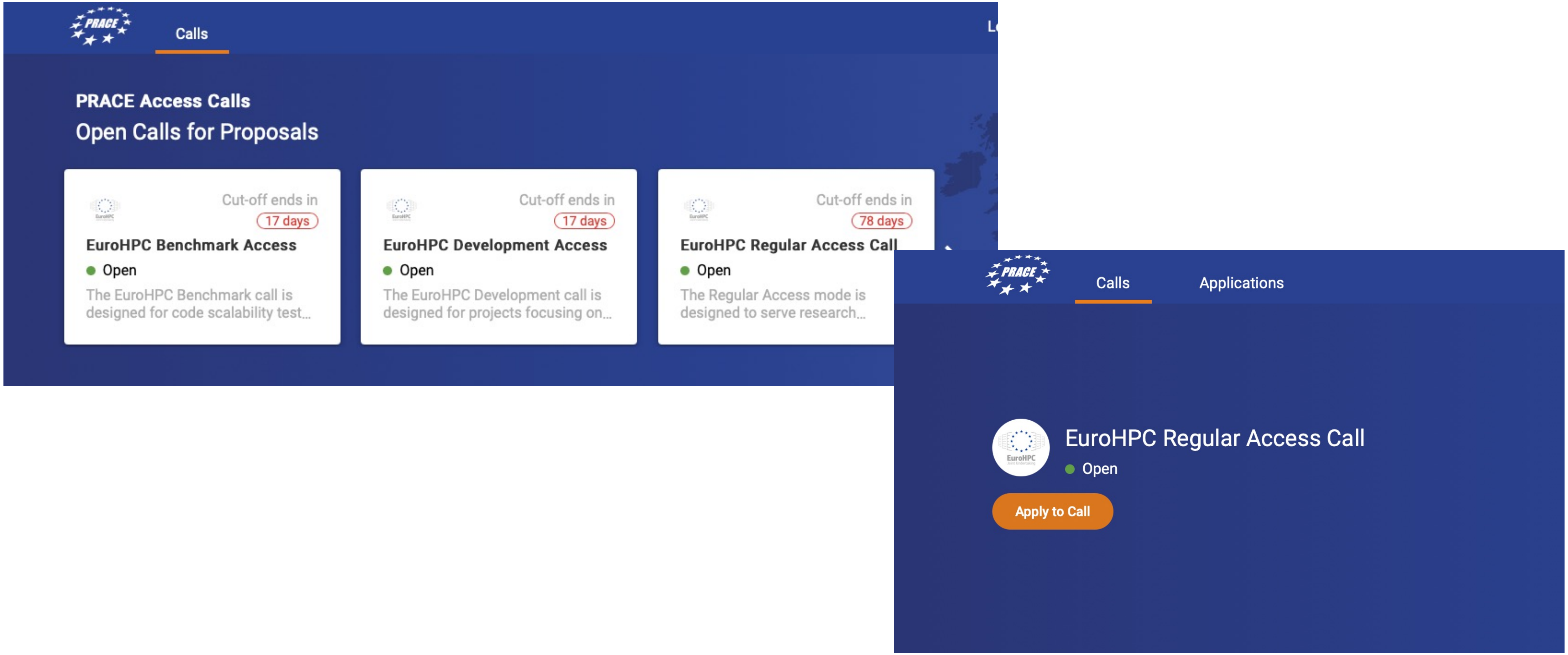
Sistems/Partitions

System/Partition	Benchmark		Development	
	Node Hours	Core Hours	Node Hours	Core Hours
VEGA CPU	5 000	640 000	10 000	1 280 000
VEGA GPU	400	51 200	1 000	128 000
Discoverer	7 000	896 000	15 000	1 920 000
Karolina CPU	7 000	896 000	15 000	1 920 000
Karolina GPU	1 000	128 000	3 000	384 000
MeluXina Cluster Module – CPU	7 100	908 800	15 300	1 958 400
MeluXina Accelerator Module – GPU	1 000	64 000	3 000	192 000
MeluXina Accelerator Module – FPGA	1 500	—	5 000	—
LUMI-C	7 000	896 000	15 000	1 920 000
LUMI-G	20 000	1 280 000	N/A	N/A

BENCHMARK ACCESS CALL & DEVELOPMENT ACCESS CALL & REGULAR ACCESS CALL

Nasıl Başvurulur?

Online Form:



https://pracecalls.eu

1

Project Application

- **The Project**
- Principal Investigator
- Contact Person
- Team Members Information
- Partitions
- Development
- Special Needs
- Collaboration and Funding
- Excluded Reviewers
- Acceptance of Terms of Reference

The Project

Project details

Project title*

Project summary (abstract)*

Keywords*

☐ **Proposal for civilian purposes***

Is any part of the project confidential?*

○ Yes ○ No

Project Scope and Plan document upload*

Click to choose a pdf | **Browse**

The file must be in a PDF format

Research fields

Research field title*

Research field share (%)*

The sum of all research fields should not exceed the total of 100%

+ Research fields

2

Principal Investigator

Personal information

Gender*

Title*

First (given) name*

Last (family) name*

Initials

Date of birth*

E-mail address*

Secondary e-mail address

Nationality*

Phone Number

+32

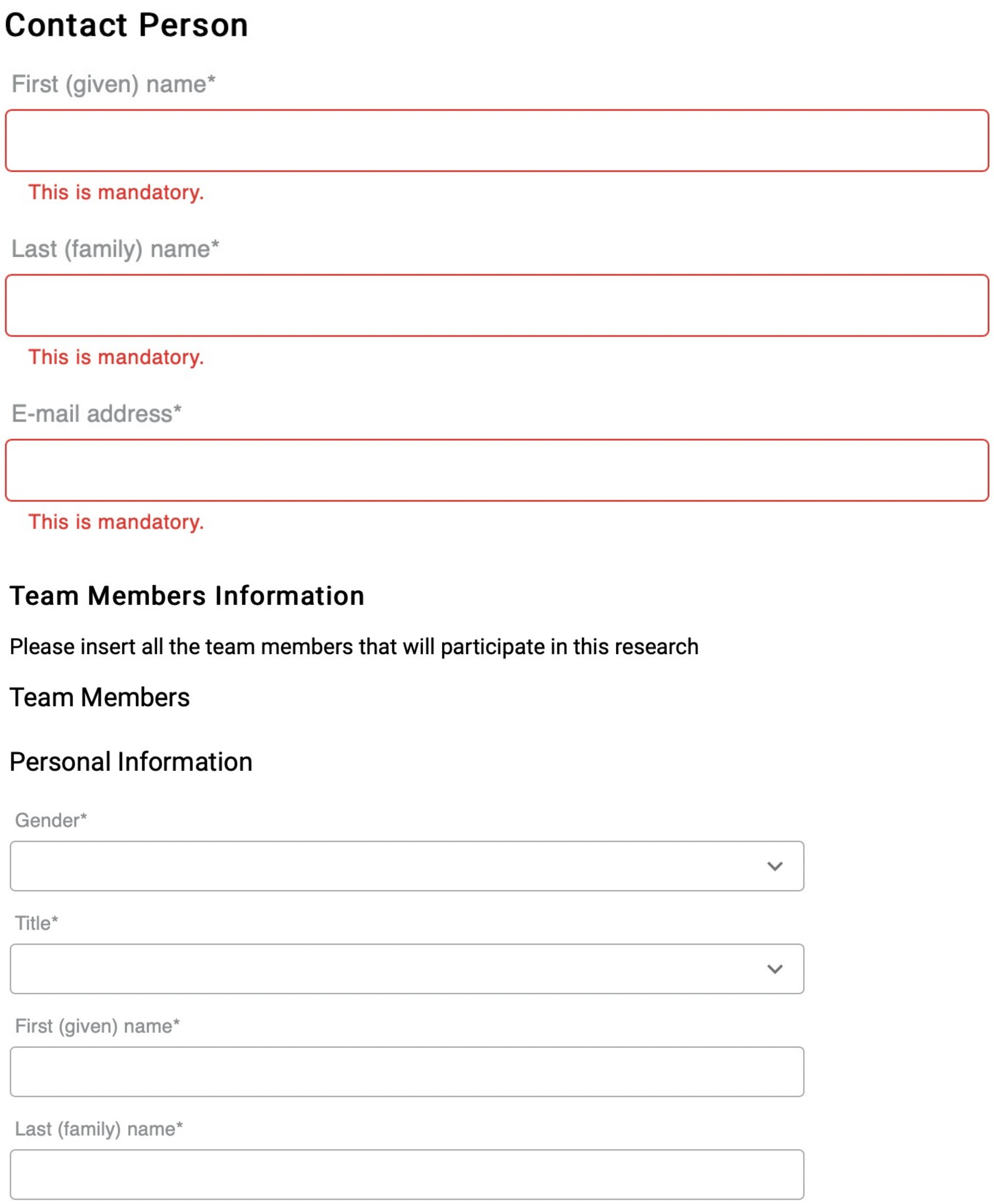
Job title*

☐ **Employment contract valid for more than 3 months after end allocation***

Website

Organization details

3



Contact Person

First (given) name*

This is mandatory.

Last (family) name*

This is mandatory.

E-mail address*

This is mandatory.

Team Members Information

Please insert all the team members that will participate in this research

Team Members

Personal Information

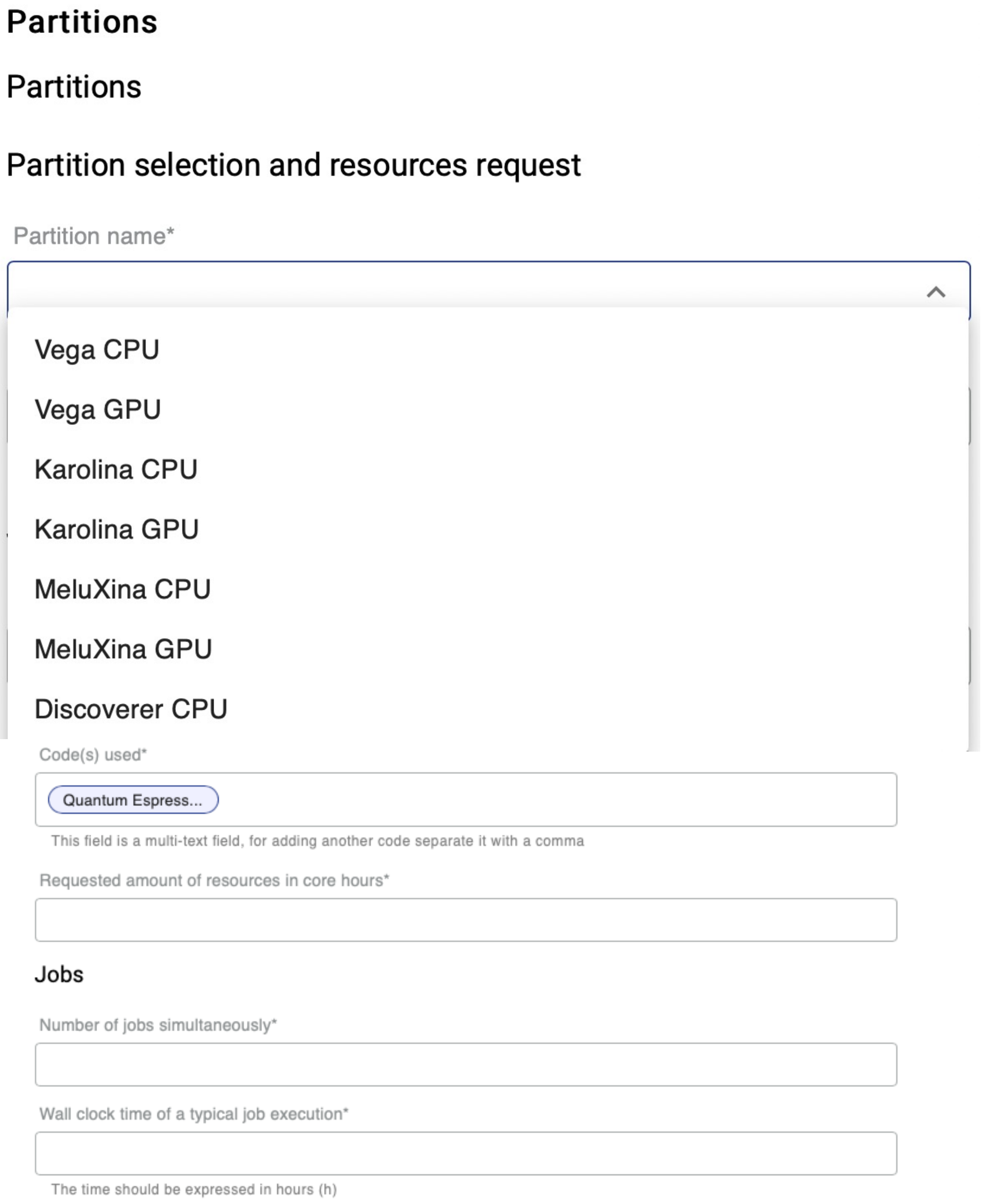
Gender*

Title*

First (given) name*

Last (family) name*

4



Partitions

Partitions

Partition selection and resources request

Partition name*

Vega CPU

Vega GPU

Karolina CPU

Karolina GPU

MeluXina CPU

MeluXina GPU

Discoverer CPU

Code(s) used*

Quantum Espress...

This field is a multi-text field, for adding another code separate it with a comma

Requested amount of resources in core hours*

Jobs

Number of jobs simultaneously*

Wall clock time of a typical job execution*

The time should be expressed in hours (h)

Checkpoints

Are you able to write checkpoint?*

◯ Yes ◯ No

Maximum time between 2 checkpoints*

The time should be expressed in hours (h)

Core

Minimum # cores*

Average # cores*

Maximum # cores*

Memory

Minimum job memory*

Total usage over all cores GB

Average job memory*

Total usage over all cores GB

Maximum job memory*

Total usage over all cores GB

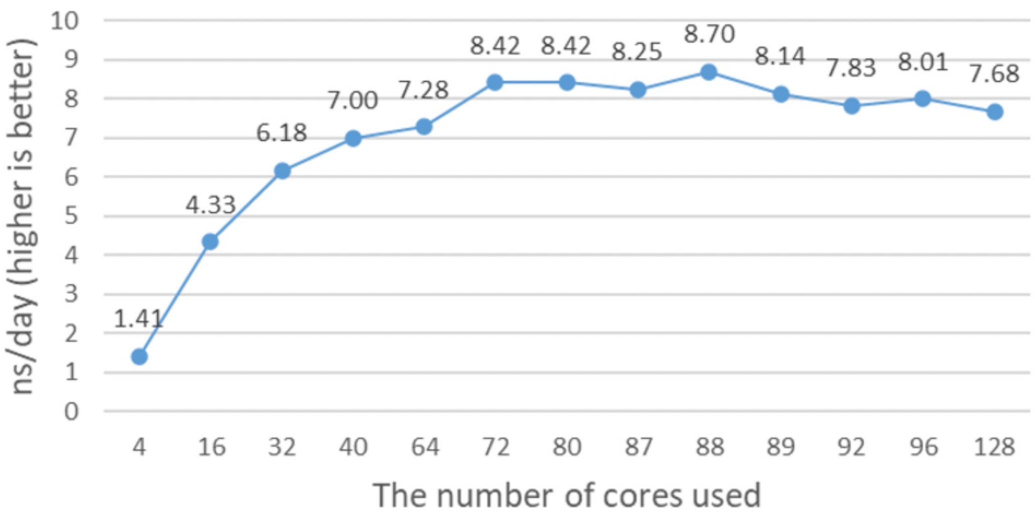
4

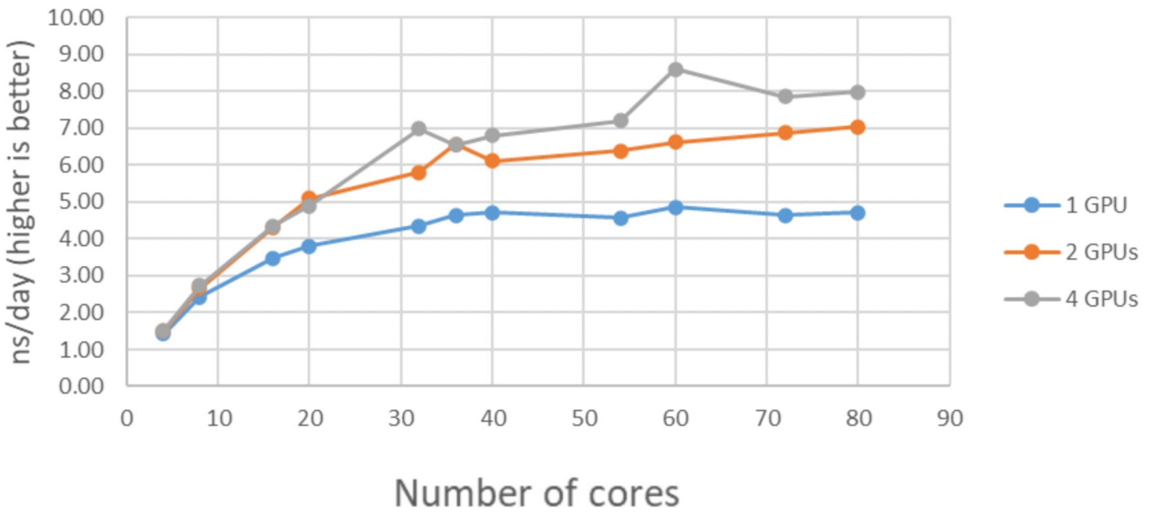
Örnek

4

NAMD

4x NVIDIA A100 GPU. 3 milyon atomdan oluşan sistem





[1] https://infohub.delltechnologies.com/p/molecular-dynamics-simulations-with-dell-emc-poweredge-xe8545-server-and-nvidia-a100/

Development

5

The Development tab should include the following: description of main algorithms, how they have been implemented and parallelized, and their main performance bottlenecks and the solutions to the performance issues you have considered. For each code that needs to be optimized, please provide the details below. Codes can be added by clicking on the Add code button.

Development of the code(s) description*

This is mandatory.

Code details

Name and version of the code

Webpage and other references

Licensing model

Contact information of the code developers

Your relationship to the code (e.g. developer, collaborator to main developers, etc.)

Special Needs

6

Please specify the needs that are not listed and are specific and necessary for the completion of the project (e.g. data transfer tools, workflow tools, other middleware requirements, dependence on a specific member of local/external staff, funding stream, 3rd party software, outcomes of other projects, etc.)

Special needs description*

Collaboration and Funding

7

Please mention any additional funding or international collaborations that you are involved in. This will help strengthen your submission.

In addition, any information on international collaborations that you are involved in will help the PRACE Communications team in their dissemination activities to promote your work should you be awarded.

Select one or more funding options applicable to the project*

BENCHMARK ACCESS CALL & DEVELOPMENT ACCESS CALL & REGULAR ACCESS CALL

Çevrimiçi Form:

- Doküman adı: Project Scope and Plan – Regular Access
- Online olarak doldurulan forma oldukça benzer, sayfa sayısı vb. ayrıntılar yer alır.

1

Project name	
Research field	

Principal Investigator (PI)

Title (Dr., Prof., etc.)	
First (given) name	
Last (family) name	
Organisation name	
Department	
Group	
Country	

Co-PIs (same information)

Provide the details of any Co-PIs in the project, including Title, First (given) name, Last (family) name, Organisation, Department, Group and Country.

It is mandatory to include all team members on the online form.

Co-Principal Investigator (Co-PI)

Title (Dr., Prof., etc.)	
First (given) name	
Last (family) name	
Organisation name	
Department	
Group	
Country	

2

Bölümler

1 Key scientific/societal/technological contribution of the proposal (200 words max.)

Outline the scientific/societal/technological importance of your project, how High Performance Computing (HPC) will help you achieve your goals and what the major expected outcomes are. This section would typically be the same as the abstract of the proposal in the submission form.

<Enter your text here>

2 Detailed proposal information (Maximum 8 pages, graphs and tables included)

The information should be suitable for expert peer review in your discipline. It must also have appropriate information for a broader audience as your proposal will be evaluated by a panel and in parallel with proposals in other disciplines.

2.1 Justification for the importance of the scientific problem and the requested resources (1 page)

Describe the proposed research and the main scientific/technical advances you will achieve with the requested EuroHPC allocation. For industrial applications, proposals should demonstrate the innovation and industrial impact on the specific market and the broader socio-economic impact. For public sector applications, the proposal should demonstrate the innovative aspects of the applications, the expected societal impact, and how the application will contribute to the delivery of quality and efficient public sector services. The justification of the requested resources must be clearly linked to the software performance evaluation (Section 2.6).

<Enter your text here>

2.2 Overview of the project (2 pages)

Describe the motivation, objectives and scientific challenges of the problem. Describe and justify the choice of computational methods. State the advances that will be enabled through the requested EuroHPC Regular Access award (e.g. impact on community paradigms, valuable insights or solving a long-standing challenge, new technology/therapy, etc.). Provide a list of expected outcomes of your proposal and, if relevant, the interdisciplinary value of your proposal.

<Enter your text here>

2.3 Validation, verification, state of the art (1 page)

Please describe the validity of the simulations and predictions made with this proposal. In case you provide references to relevant publications please include here also the key relevant results. Please address issues of reproducibility and highlight the predictive capabilities of your simulations.

2.3.1 Validation & Verification

Please summarize the validation of your model against experiments or other established reference data. Please also provide how the numerical consistency and stability of your computational method has been verified or provide evidence of existing verifications.

<Enter your text here>

https://prace-ri.eu/call/eurohpc-ju-call-for-proposals-for-regular-access-mode-2023-03-03-cutoff/

BENCHMARK ACCESS CALL & DEVELOPMENT ACCESS CALL & REGULAR ACCESS CALL

2

2.4 Software and Attributes (1 page)

*(Please see also **Examples of Performance Reporting** in Section 2.6.2.1). Describe the software that will be used including a discussion of the state of the art in the field. The description should mention:*

2.4.1 Software

Please describe all codes you are using in the proposal. Justify your choices and describe alternatives (if any).

<Enter your text here>

2.4.2 Particular libraries

Describe particular libraries required by the production and analysis software, algorithms and numerical techniques employed (e.g. finite element, iterative solver), programming languages. Please specify requirements for compilation or build environment (build system (e.g. cmake, python version), version control system (e.g. git, subversion) etc.).

<Enter your text here>

2.4.3 Parallel programming

Model(s) used (e.g., MPI, OpenMP/Pthreads, CUDA, OpenACC, etc.).

<Enter your text here>

2.4.4 I/O requirements

I/O requirements (e.g. amount, size, bandwidth, etc.) for execution, input files, restart and other output. Describe I/O strategy (number of files, frequency, read/write size) and I/O behaviour of your code during the period of calculations. Please specify the restart overhead, not only for I/O: (e.g. a code may have to perform a costly domain decomposition first).

<Enter your text here>

2.6 Performance of Software (Maximum 2 pages)

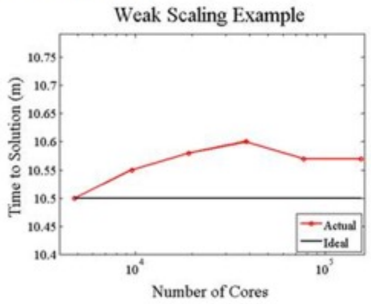
2.6.1 Testing of your code on the requested machine

2.6.2 Quantify the HPC performance of your project

*The presented data must be representative of the entire workflow of the project proposed and refer to the main application code you intend for the production work. The software scalability data (see Examples of **Performance Reporting** below) must be used to choose the most efficient job size(s) for the simulations planned in production: the corresponding software performance must be clearly linked to the justification of the*

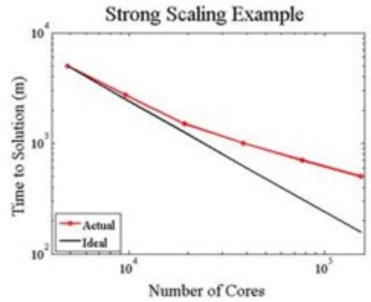
2.6.2.1 Strong and weak scalability

Weak Scaling Example



nProc	Time to Solution (m)	Ideal Time to Solution (m)
4800	10.50	10.50
9600	10.55	10.50
19200	10.58	10.50
38400	10.60	10.50
76800	10.57	10.50
153600	10.57	10.50

Strong Scaling Example



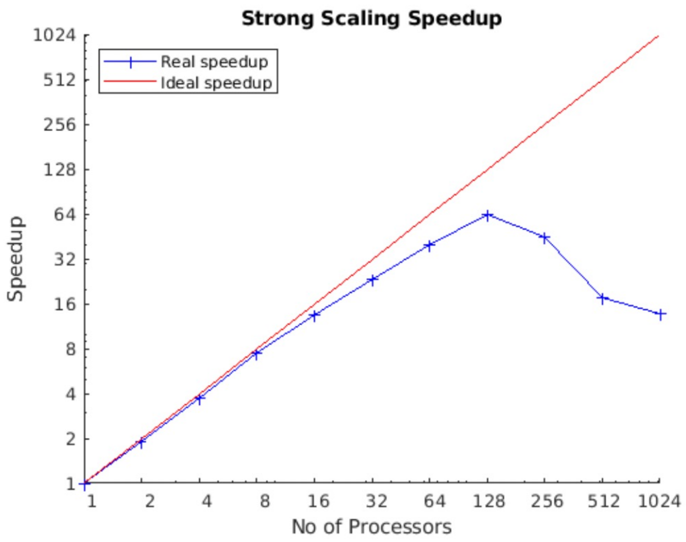
nProc	Time to Solution (m)	Ideal Time to Solution (m)
4800	5000.00	5000.00
9600	2725.00	2500.00
19200	1500.00	1250.00
38400	1000.00	625.00
76800	700.00	312.50
153600	500.00	156.25

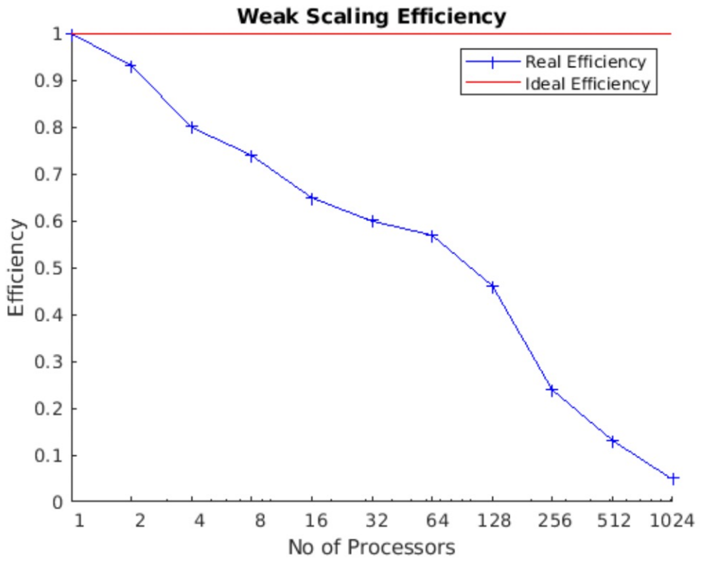
Scalibility (Ölçeklenebilirlik)

- Yüksek performanslı bilgi işlem kümeleri ile çok sayıda işlemci kullanarak büyük problemler çözülebilir.
- Çok sayıda işlemcinin, hesaplama süresini azaltmak için aynı anda çalıştığı parallel hesaplama durumları olabilir.
- Bu durumda donanım ve yazılımın kaynak miktarı arttığında daha fazla hesaplama gücü sağlama yeteneğini belirtmek için kullanılır.

Strong Scaling ve Weak Scaling

- Strong scaling: İşlemci sayısı artırılırken, problemin boyutu sabit tutulur.
- Weak scaling: Hem işlemci sayısı hem de problemin boyutu artırılır.
- Her iki durumda da, simülasyon ya da deneyin süresi CPU çekirdeği sayısının bir fonksiyonu olarak ölçülür.





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<Enter your text here>

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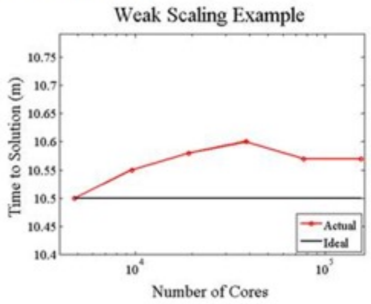

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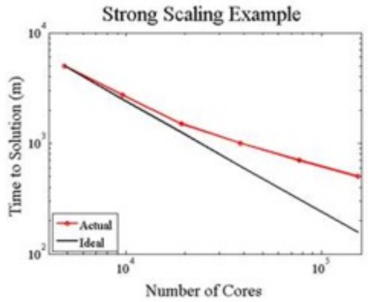
Strong Scaling Example



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76800	700.00	312.50
153600	500.00	156.25

Not: Hedef sistem ve teklifte bulunacağınız sistem birbirinden farklı olduğunda; hazırlık testlerinin yapıldığı makineden istenen sisteme dönüştürme faktörünü (Time to Solution ve Normalized Total Time to Solution) belirtmeniz beklenmektedir.

Time to Solution

$$T_i^{*} = t_i \,.\, N_c \,/\, N_e$$

Normalized Total Time to Solution

$$T_f^{*} = t_f \,.\, N_c \,/\, N_e$$

t_i → yineleme başına süre (the time per iteration)
t_f → toplam çözüm süresi (the total time to solution)
N_c → çekirdek sayısı (the number of cores)
N_e → Hesaplama öğelerinin sayısı (the number of computational elements)

3 Milestones (quarterly basis) (Maximum 1 page)

3

Run Type	Code(s)	No. of runs	No. of nodes	No. of steps per run	Time per step(s)	Total node hours
A (init. condition prep.)	Code 1					
B (low resolution)	Code 2					
C (high resolution)	Code 2					
D (post processing)	Code 3					

3.1 Gantt Chart

Provide a Gantt Chart of the simulation plan in production indicating job sizes and scheduling of computing tasks including a communication plan for the results and the strategy and timeline for the dissemination of the results.

<Enter your text here>

4 Personnel and Management Plan (0,5 page)

4

What personnel are already in place and what are their roles on the project? If applicable, describe (i) personnel that will be hired for the project in the future and their responsibilities and (ii) potential personnel turnover that may occur during the project and a strategy for replacing them. The EuroHPC Regular Access calls welcome proposals from individual PIs or teams of collaborators. Outline the focus of each individual or subgroup and their interrelationships.

It is mandatory to include all team members on the online form.

5 References (Maximum 30)

5

<Enter your text here>

6 Confidentiality (0,5 page)

6

- Is any part of the project covered by confidentiality? **yes/no**

Teşekkürler…