



Turkish National Science e-Infrastructure (TRUBA)

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TÜBİTAK ULAKBİM
Network Technologies Department
TRUBA Team

09 APRIL 2025



EuroCC4SEE & BioExcel Training

Exploring Biomolecular Modeling & Simulations

Hybrid (online & onsite: SabancıDx Digital Campus, İstanbul))
April 9-10, 2025

Free participation

OUTLINE

01 | High Performance Computing
Resources & Architecture

02 | TRUBA Projects

03 | Usage of TRUBA

04 | Connection to TRUBA

05 | Example of SLURM Script

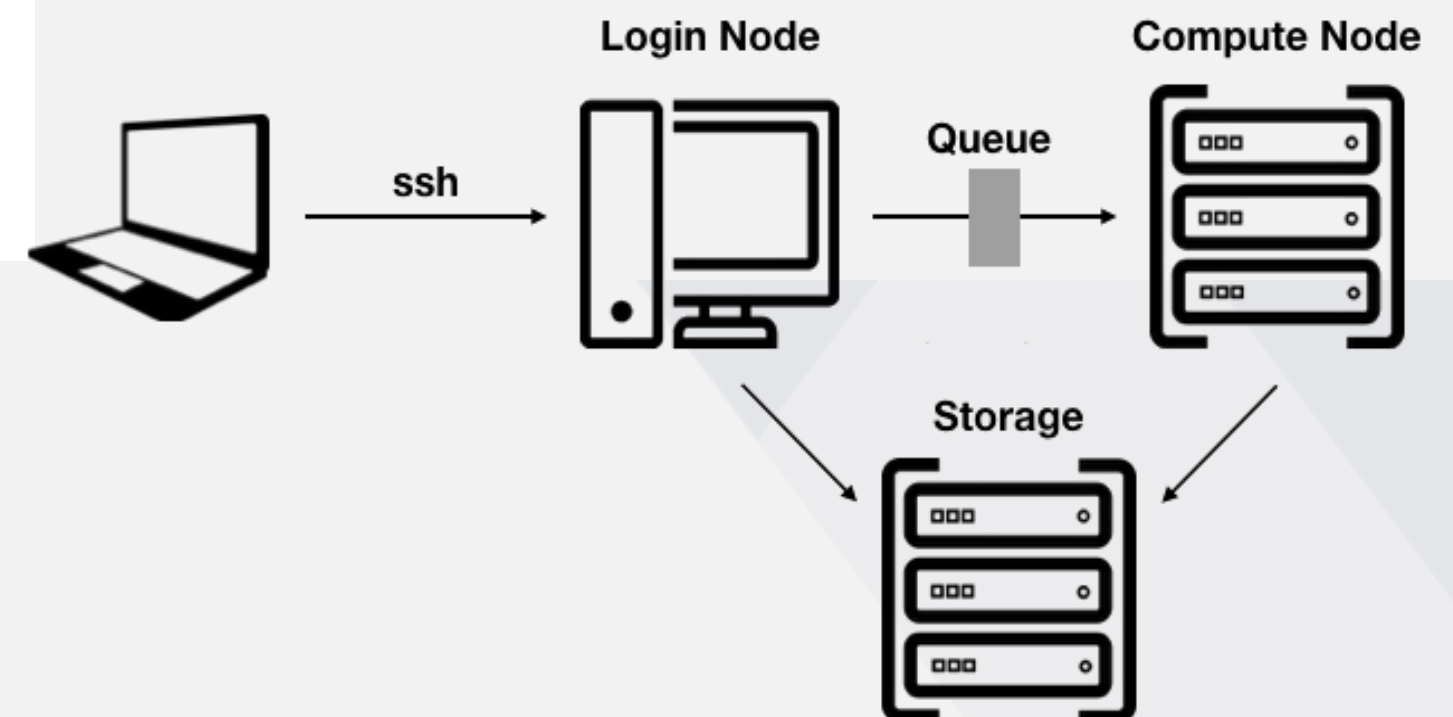
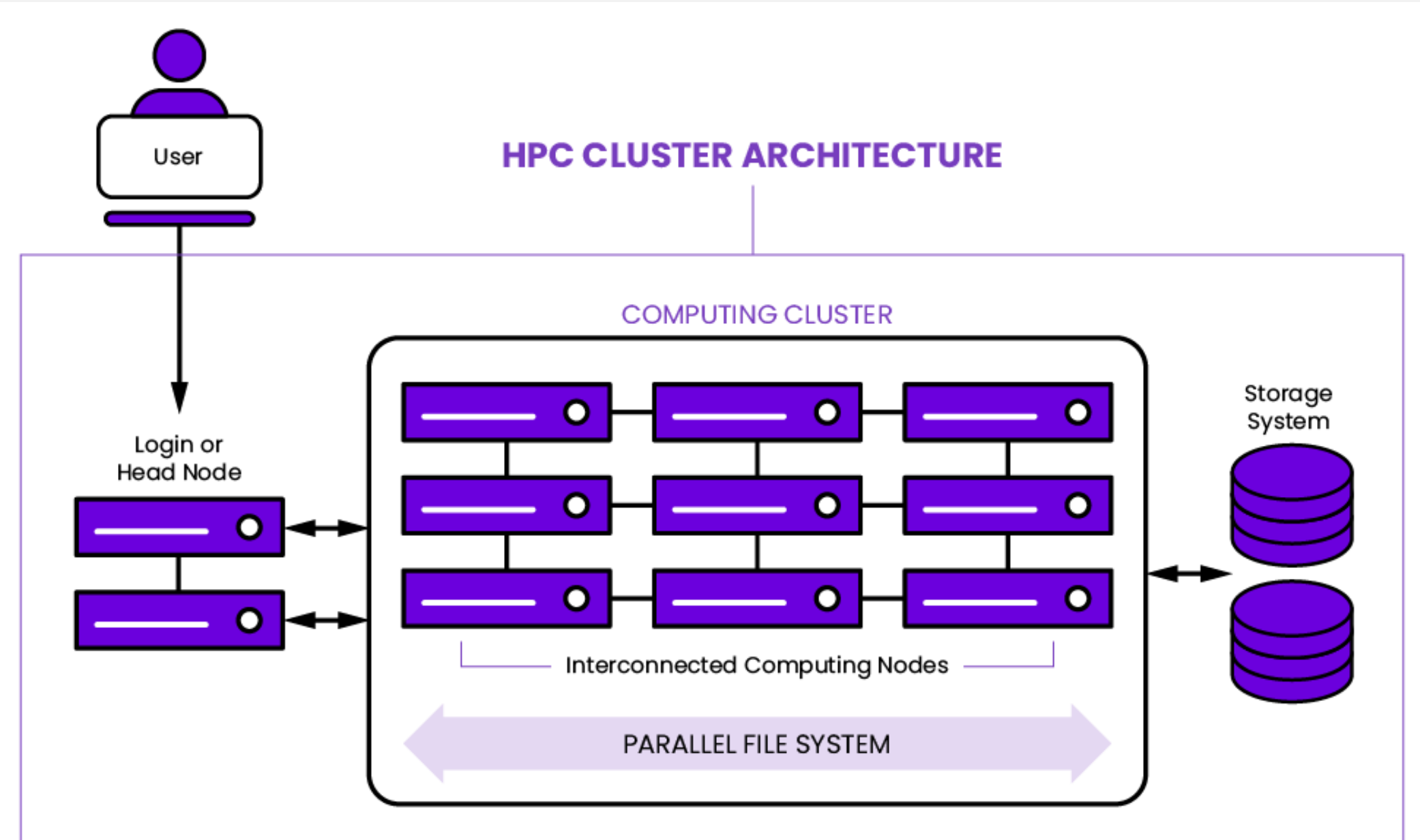


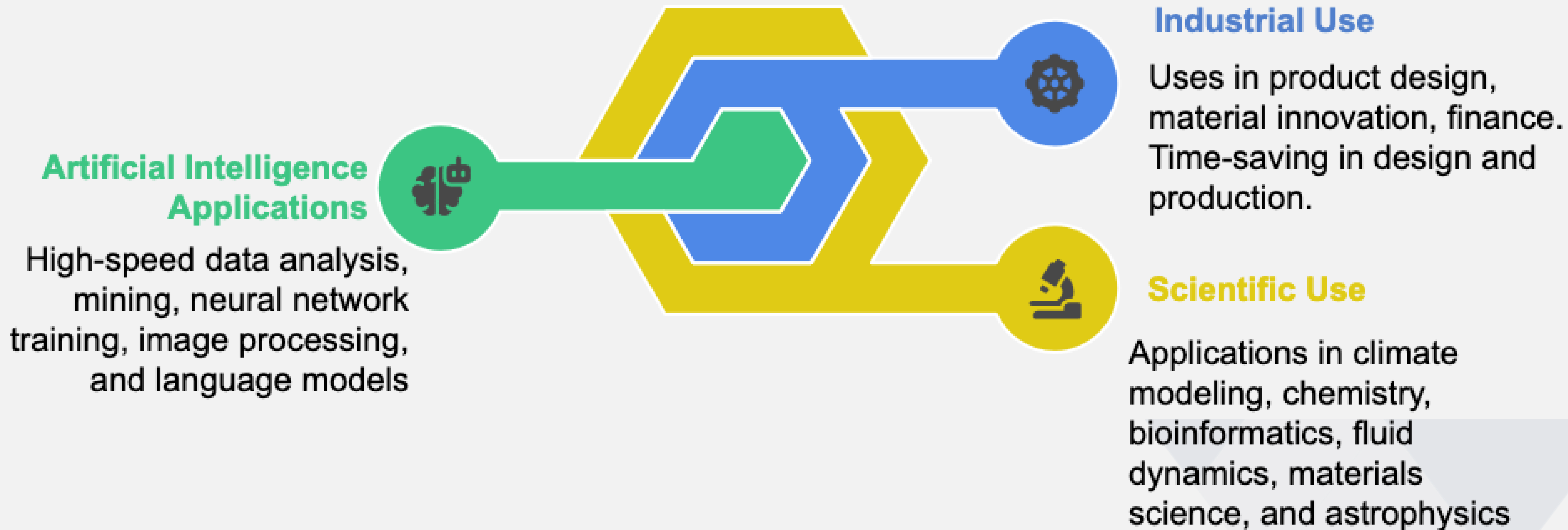
High Performance Computing Resources

- Computer systems with very high performance.
- Systems that combine the power of multiple computers to get much higher computing power from a desktop/laptop computer.
- This can solve big problems in science, engineering and business.

• The ARF Compute Cluster = 35.000 laptops

High Performance Computing (HPC) is the use of parallel processing techniques to solve complex and large-scale problems on supercomputer infrastructures that cannot be solved by laptop/desktop computers.





TRUBA's Strategic Initiatives Overview

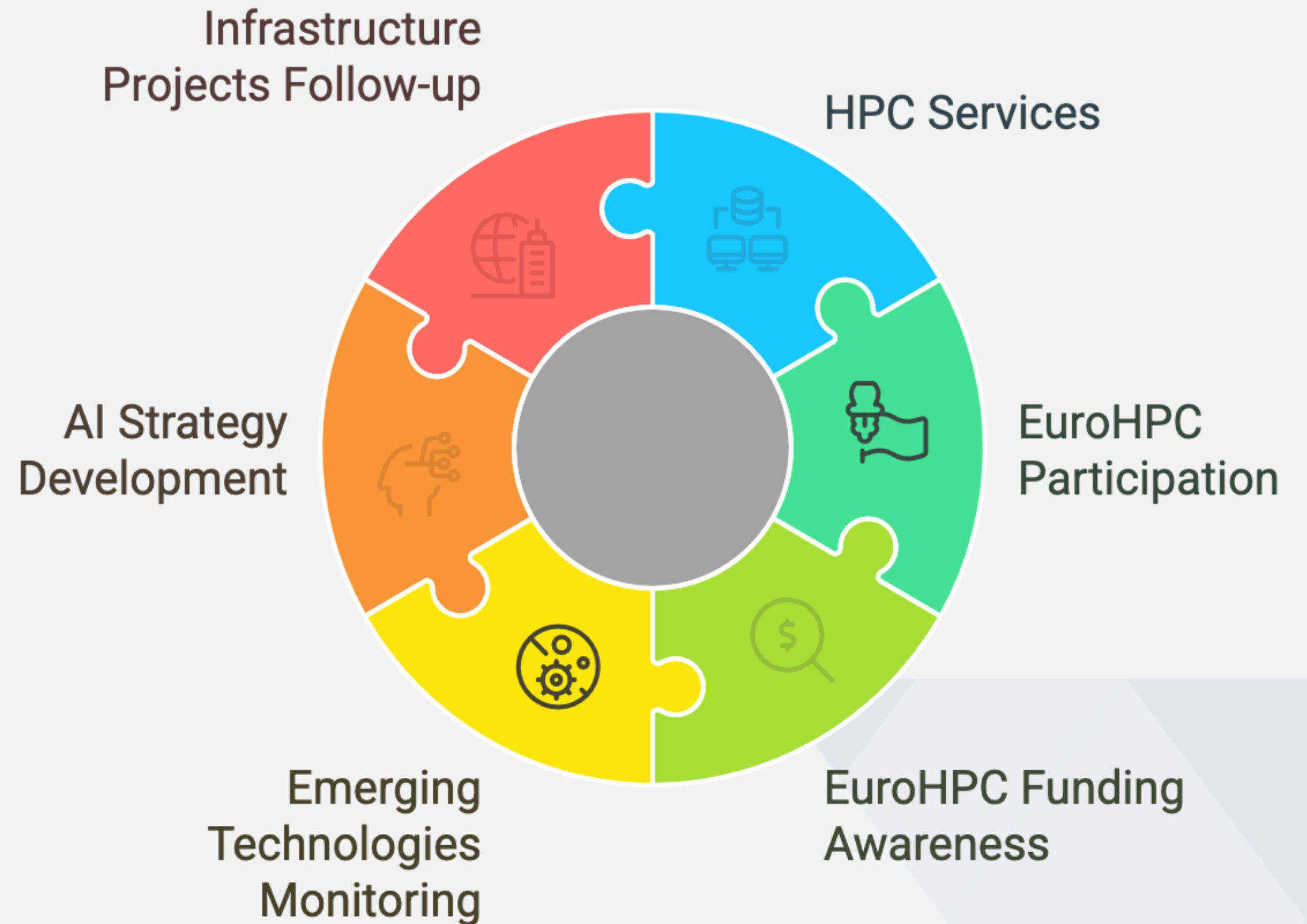
Operated by: TÜBİTAK ULAKBİM

Target Users:

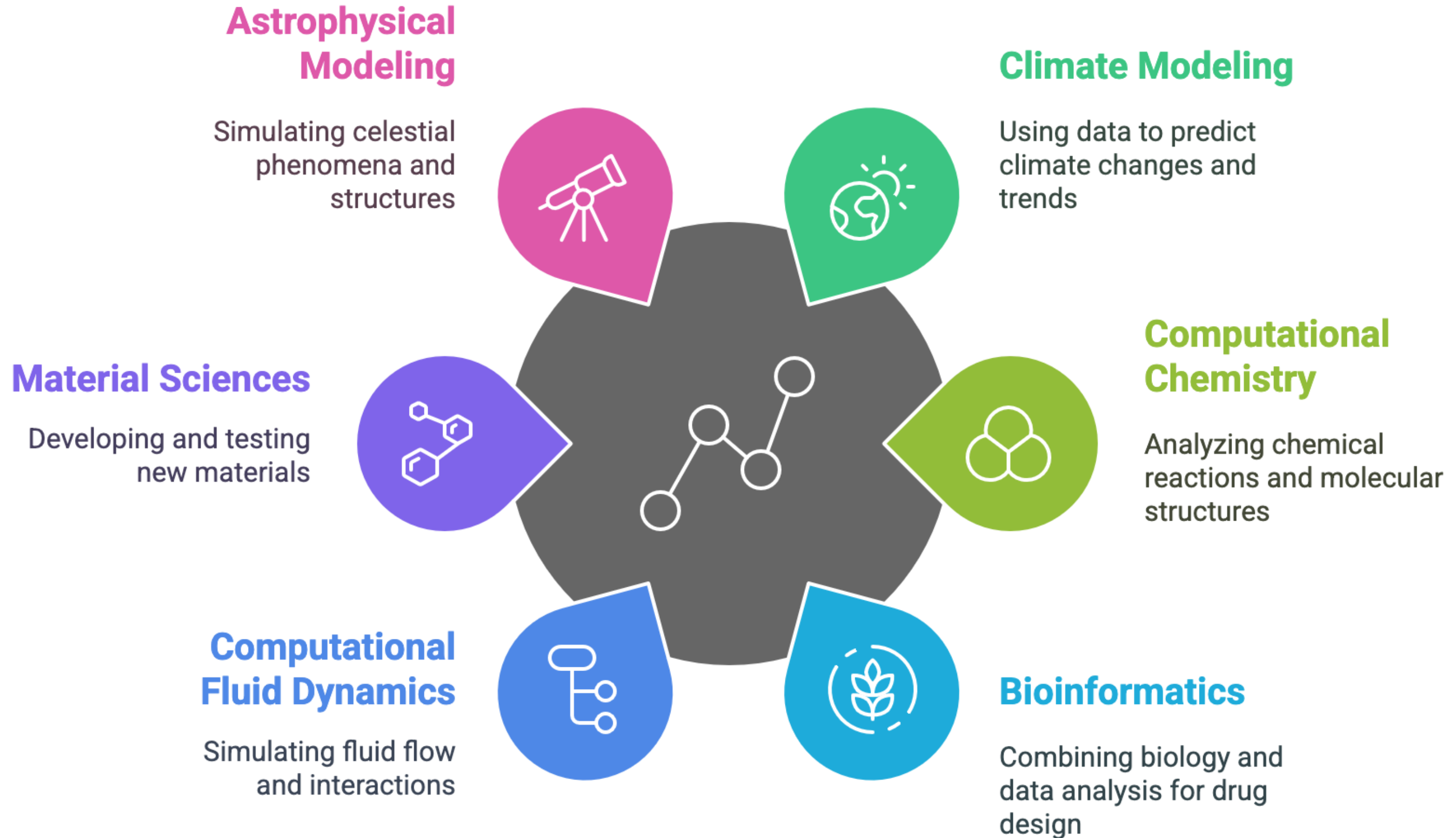
- Academic researchers
- Public institutions
- Industry professionals

Core Mission:

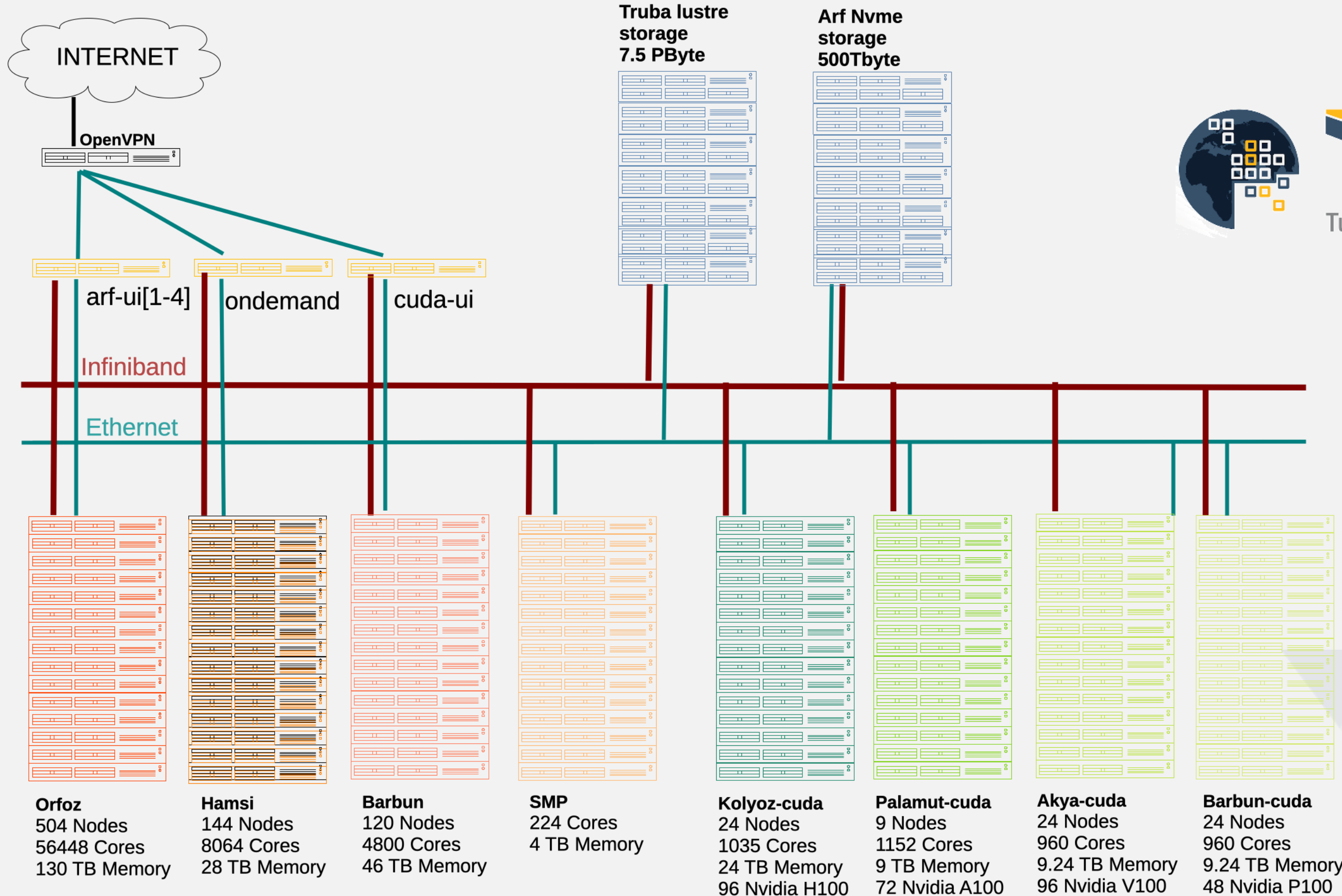
- Support **cutting-edge scientific research** and innovation
- Enable access to **high-performance computing resources**



Applications of Advanced Computational Techniques



TRUBA - Turkish National Science e-Infrastructure



TRUBA
Turkish Science e-Infrastructure

Calculation Nodes	Year	#Nodes	Architecture	Processor	Performance (1 Node)	Memory (1 Node)
Orkinos	2016	1	14 çekirdek x 16 CPU	Xeon E7-4850 v3 2.20GHz	7900Gflops	4 TB
Barbun	2018	120	20 çekirdek x 2 CPU	Xeon Scalable 6148 2.40GHz	2048Gflops	384 GB
Hamsi	2021	144	28 çekirdek x 2 CPU	Xeon Gold 6258R 2.70GHz	4800Gflops	192 GB
Orfoz	2023	504	56 çekirdek x 2 CPU	Intel(R) Xeon(R) Platinum 8480+ 2.0GHz	6900Gflops	256 GB

<https://docs.truba.gov.tr/TRUBA/kullanici-el-kitabi/hesaplamakumeleri.html>



TRUBA – Top500 & Green500 Certificates



ARF - ThinkSystem SD650 v3, Xeon Platinum 8480+ 56C 2GHz, Infiniband NDR200

TRUBA, Turkey

is ranked

No. 354

among the World's TOP500 Supercomputers

with 3.00 PFlop/s Linpack Performance

in the 64th TOP500 List published at the SC24

Conference on November 19, 2024.

Congratulations from the TOP500 Editors



ARF ACC - ThinkSystem SD650-N V3, Xeon Gold 6548Y+ 32C 2.5GHz, NVIDIA H100 80GB HBM3,

Infiniband NDR200, Rocky Linux 9.4

TRUBA, Turkey

is ranked

No. 227

among the World's TOP500 Supercomputers

with 4.36 PFlop/s Linpack Performance

in the 64th TOP500 List published at the SC24

Conference on November 19, 2024.

Congratulations from the TOP500 Editors



ARF ACC - ThinkSystem SD650-N V3, Xeon Gold 6548Y+ 32C 2.5GHz, NVIDIA H100 80GB HBM3,

Infiniband NDR200, Rocky Linux 9.4

TRUBA, Turkey

is ranked

No. 26

among the World's TOP500 Supercomputers

with 52.547 GFlops/watts Performance

in the Green500 List published at the SC24

Conference on November 19, 2024.

Congratulations from the Green500 Editors



TRUBA
Turkish Science e-Infrastructure

Who can use TRUBA?

- ❑ Academic Researchers: Including faculty members, PhD candidates, postdoctoral researchers, and Master's students (with advisor approval).
- ❑ Researchers from Public Institutions: Government-affiliated researchers are eligible.
- ❑ Industry Researchers: Professionals from companies **established or located in Türkiye**



How to Apply?

- ❑ Register: Visit <http://portal.truba.gov.tr> to begin the application process.
- ❑ Verification: The researcher's identity is verified through e-Government and YÖKSİS.
- ❑ Access Credentials: Upon approval, login credentials (username and password) are provided to the researcher through TRUBA portal.



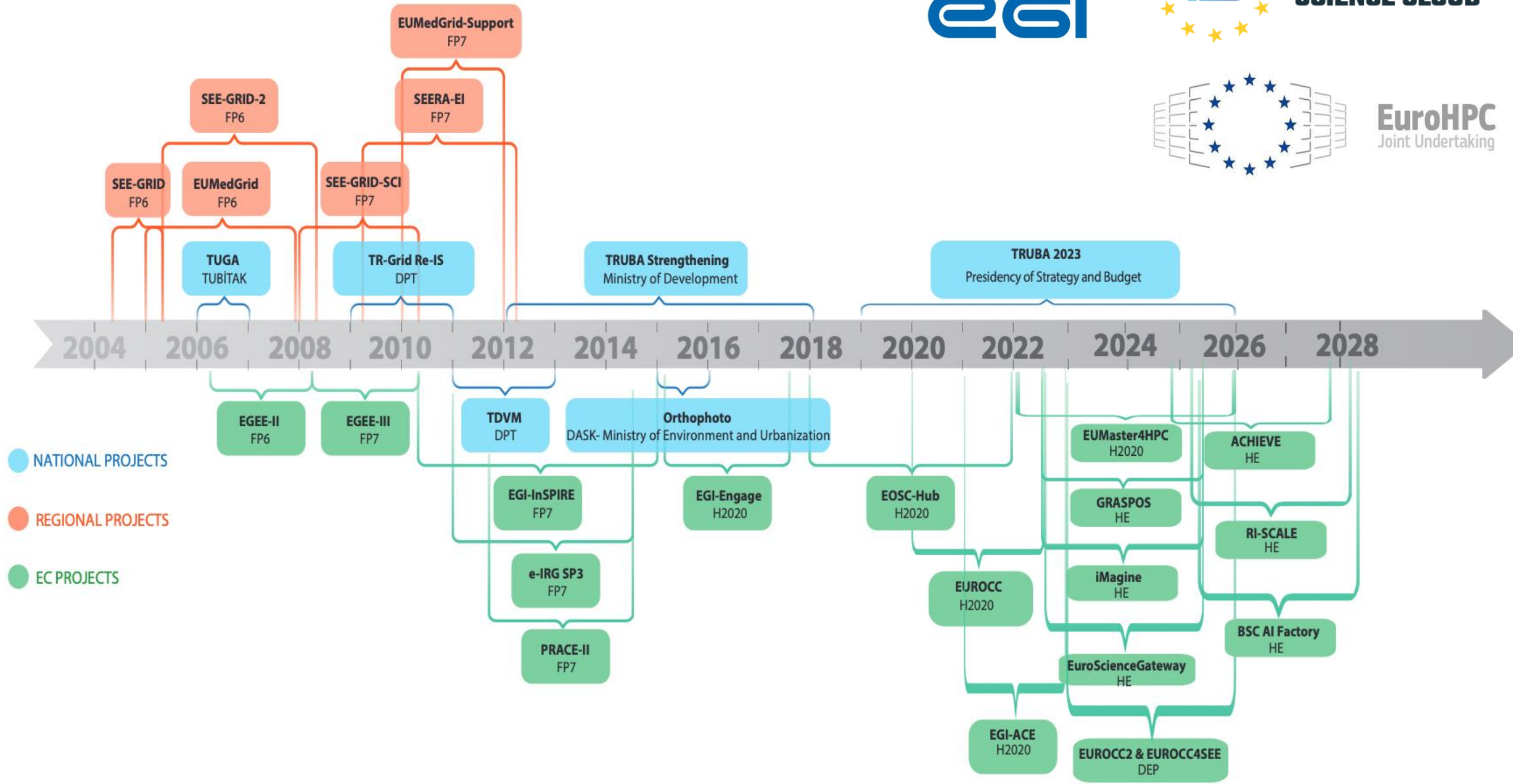
grid-teknik@ulakbim.gov.tr

ardeb@ulakbim.gov.tr



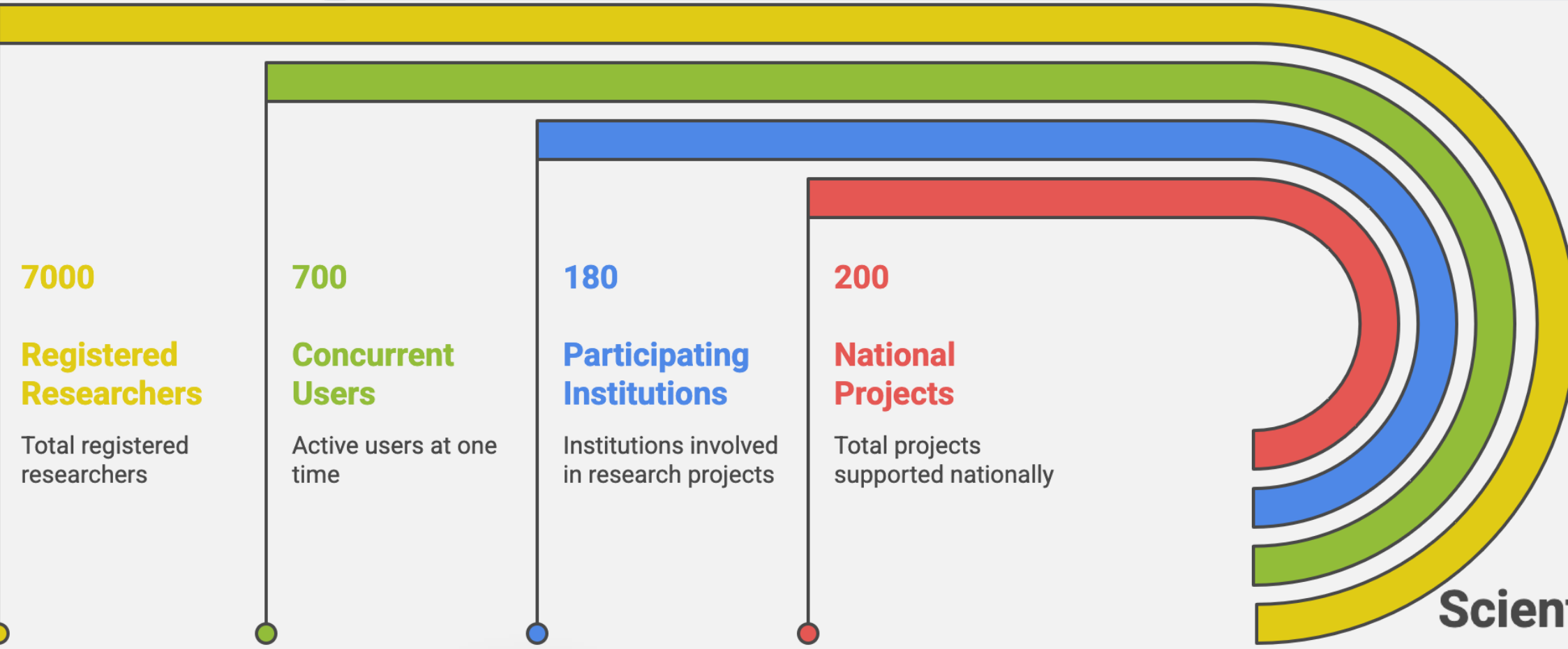
TRUBA
Turkish Science e-Infrastructure

TRUBA Projects



- 27 EU Project
- 3 EU Formation Membership

TRUBA Usage Metrics



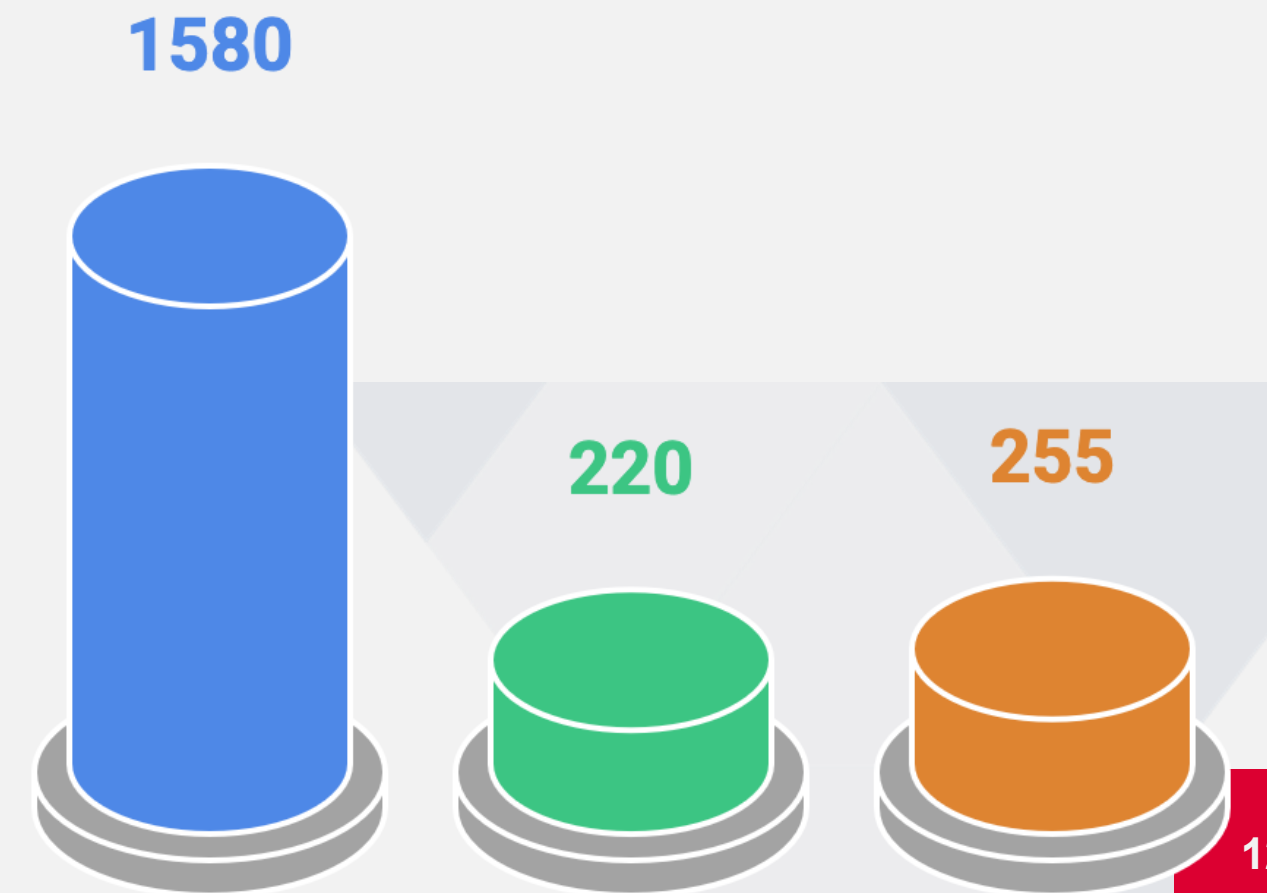
Scientific Outputs Using TRUBA Resources



Articles
Research publications using TRUBA resources

Theses
Graduate research projects utilizing TRUBA

Presentations
Conference contributions by TRUBA researchers



Basic Linux Knowledge

- ❑ Linux basic structure
- ❑ File, directory structure
- ❑ User permissions on files and directories
- ❑ Basic shell commands
- ❑ File operations, file editing
 - (cp, mv, mkdir, cd, find, vi, etc.)
- ❑ Connection and file transfer
 - (ssh, scp, sftp, etc.)
- ❑ X-forwarding

<https://docs.truba.gov.tr/>

Application Knowledge

- ❑ What/How does it calculate?
- ❑ How it works (serial, MPI, OpenMPI)
- ❑ Dependency on other applications and libraries
- ❑ Installation/Compilation processes
- ❑ Structuring according to the problem
- ❑ Input and output files
- ❑ Amount of resources needed



TRUBA Kullanıcı Dokümanları

Hızlı Erişim

- Duyurular
- ARF
- Yüksek Performanslı Dosya Sistemleri
- OpenVPN Bağlantısı
- SSH ile Bağlantı
- Open OnDemand Arayüzü
- Kullanıcı El Kitabı
- Sıkça Sorulan Sorular
- TRUBA Ekibiyle İletişim Kurmak için Şablonlar
- TRUBA Başlangıç Seminerleri

Öğretici Başlangıç Materyalleri

- TRUBA Sisteminde Çok Kullanılan Linux Komutları
- TRUBA Kümelerini İlk Kez Kullanacaklar İçin

ARF Hakkında

- ARF Hesaplama Kümesi
- Gaussian

Uygulama Kılavuzları

- TRUBA'da Uygulama/Kütüphane Kurulumu
- Python Kılavuzu
- R Kılavuzu
- GPU Kılavuzu
- Derin Öğrenme Kılavuzu
- Veri Analitiği Kılavuzu
- Amber Kılavuzu
- CASTEP Kılavuzu
- Gaussian Kılavuzu
- GROMACS Kılavuzu
- LAMMPS Kılavuzu
- Quantum Espresso Kılavuzu
- VASP Kılavuzu
- MATLAB Kılavuzu
- Snakemake Kılavuzu
- CVMFS Kullanımı
- Apptainer Kılavuzu

TRUBA Hakkında

- Türk Ulusal Bilim e-Altyapısı (TRUBA)
- Yüksek Performanslı Dosya Sistemleri
- TRUBA Mimarisi
- Open OnDemand Arayüzü
- Kullanıcı El Kitabı
- Sıkça Sorulan Sorular
- Proje Kapsamında TRUBA HSB ve VSB hizmetleri
- Yapılan Çalışmalarda TRUBA'ya Türkçe ve İngilizce Teşekkür Örnekleri
- TRUBA Topluluk Portalı

EuroHPC Hakkında

- EuroHPC Ortak Girişimi
- EuroHPC Sistemleri
- EuroHPC Sistemlerine Erişim Modları ve Çağrılar
- Inno4scale Çağrısı

Eğitim Materyalleri

- Büyük Veri
- OpenMP
- OpenMPI
- PyTorch
- CUDA
- Keras
- Kuantum Hesaplama
- Hesaplamalı Akışkanlar Dinamiği (HAD)
- Hesaplamalı Temel Bilimler

Kullanıcı El Kitabı

- TRUBA Mimarisi
- TRUBA Kullanıcı Portalı
- Kullanıcı Hesapları
- Hesaplama Kümeleri
- ARF Hesaplama Kümesi
- Yüksek Performanslı Dosya Sistemleri
- Yardımcı Uygulamalar
- Yazılımlar
- Modüller
- Mevcut Uygulamalar ve Kütüphaneler
- Nümerik Kütüphaneler
- Derleyiciler
- Paralel Programlama
- Grafik Ekran Bağlantısı (X-forwarding)
- ssh X-forwarding
- TRUBA'da VNC ile Kullanıcı Arayüzlerine Görsel Bağlantı
- Yapılan Çalışmalarda TRUBA'ya Türkçe ve İngilizce Teşekkür Örnekleri
- Sıkça Sorulan Sorular
- OpenVPN Bağlantısı
- Kaynak Yöneticisi ve İş Döngüsü
- Open OnDemand Arayüzü
- TRUBA Veri Setleri
- TRUBA Topluluk Portalı

<https://docs.truba.gov.tr/>



User Support
grid-teknik@ulakbim.gov.tr



TRUBA
Turkish Science e-Infrastructure

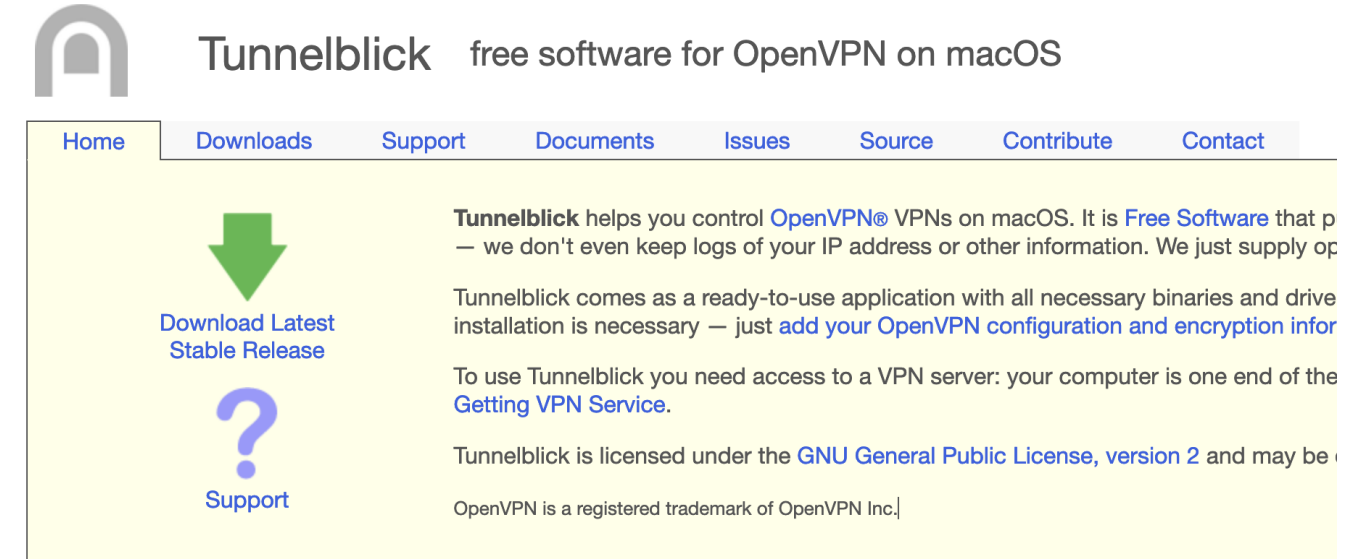
- Linux: installation through command line
 - `sudo apt-get install openvpn`

```
sevil@pop-os:~/VPN$ sudo openvpn TRUBA-genel.ovpn
2023-09-10 22:20:22 Note: Treating option '--ncp-ciphers' as '--data-ciphers' (renamed in OpenVPN 2.5).
2023-09-10 22:20:22 DEPRECATED OPTION: --cipher set to 'AES-256-CBC' but missing option --data-ciphers. Future OpenVPN version will ignore --cipher for cipher negotiations. Add 'AES-256-CBC' to --data-ciphers-fallback 'AES-256-CBC' to silence this warning.
2023-09-10 22:20:22 OpenVPN 2.5.5 x86_64-pc-linux-gnu [SSL (OpenSSL)] [LZO] [LZ4] [sqlite] [msgpack] [cryptlib]
Build on Jul 14 2022
2023-09-10 22:20:22 library versions: OpenSSL 3.0.2 15 Mar 2022, LZ4 1.9.4, LZO 2.10
Enter Auth Username: sevil
Enter Auth Password: *****
2023-09-10 22:20:29 TCP/UDP: Preserving recently used remote address: [AF_INET]193.140.99.241:1195
2023-09-10 22:20:29 UDP link local (bound): [AF_INET]193.140.99.241:1194
2023-09-10 22:20:29 UDP link remote: [AF_INET]193.140.99.241:1195
2023-09-10 22:20:29 [midye.truba.gov.tr] Peer Connection Initiated with [AF_INET]193.140.99.241:1195
2023-09-10 22:20:40 Options error: Unrecognized option or missing or extra parameter ('--ncp-ciphers') (see the manual page for OpenVPN 2.5.5)
2023-09-10 22:20:40 TUN/TAP device tun0 opened
2023-09-10 22:20:40 net_iface_mtu_set: mtu 1500 for tun0
2023-09-10 22:20:40 net_iface_up: set tun0 up
2023-09-10 22:20:40 net_addr_v4_add: 10.3.9.106/22 dev tun0
2023-09-10 22:20:40 WARNING: this configuration may cache passwords in memory -- use --write-updown-status to avoid this
2023-09-10 22:20:40 Initialization Sequence Completed
```

```
sevil@pop-os:~$ ssh sevil@172.16.7.1
sevil@172.16.7.1's password: 
```

OpenVPN – MacOS & Windows

- MacOS:
 - <https://tunnelblick.net/index.html>
 - <https://openvpn.net/client-connect-vpn-for-mac-os/>
- Windows:
 - <https://openvpn.net/community-downloads/>



Tunnelblick free software for OpenVPN on macOS

Home Downloads Support Documents Issues Source Contribute Contact

Download Latest Stable Release

Support

Tunnelblick helps you control OpenVPN® VPNs on macOS. It is Free Software that p — we don't even keep logs of your IP address or other information. We just supply op

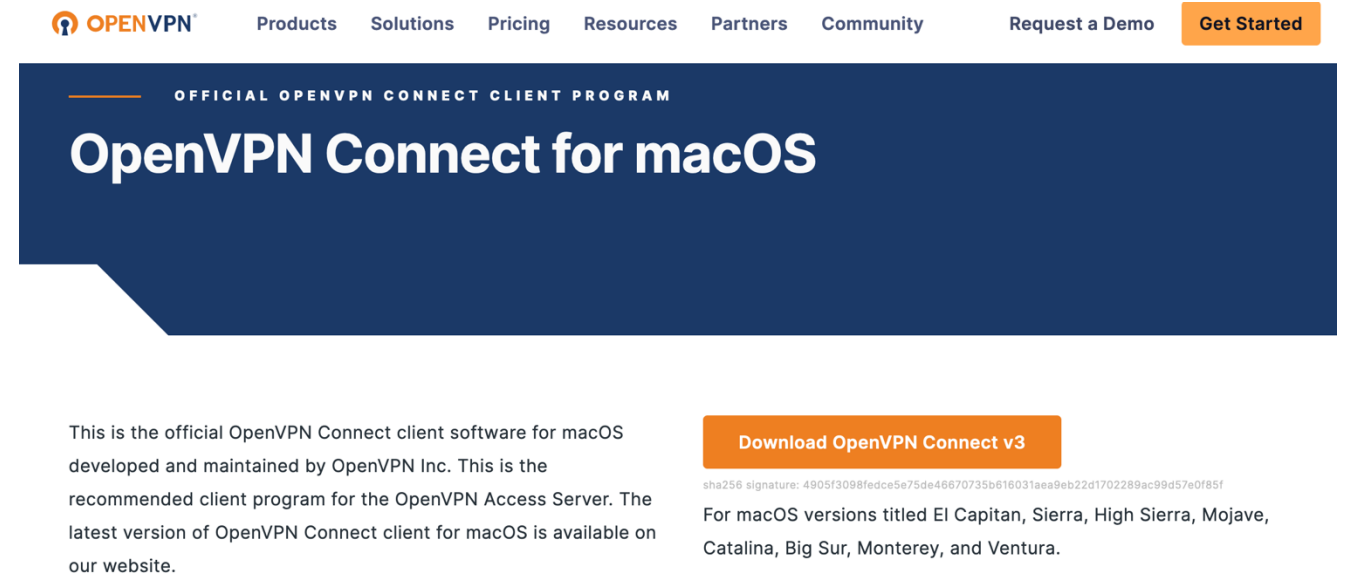
Tunnelblick comes as a ready-to-use application with all necessary binaries and drive installation is necessary — just add your OpenVPN configuration and encryption infor

To use Tunnelblick you need access to a VPN server: your computer is one end of the Getting VPN Service.

Tunnelblick is licensed under the GNU General Public License, version 2 and may be

OpenVPN is a registered trademark of OpenVPN Inc.

Windows 64-bit MSI installer	GnuPG Signature	OpenVPN-2.6.6-I001-amd64.msi
Windows ARM64 MSI installer	GnuPG Signature	OpenVPN-2.6.6-I001-arm64.msi
Windows 32-bit MSI installer	GnuPG Signature	OpenVPN-2.6.6-I001-x86.msi
Source archive file	GnuPG Signature	openvpn-2.6.6.tar.gz



OPENVPN Products Solutions Pricing Resources Partners Community Request a Demo Get Started

OFFICIAL OPENVPN CONNECT CLIENT PROGRAM

OpenVPN Connect for macOS

This is the official OpenVPN Connect client software for macOS developed and maintained by OpenVPN Inc. This is the recommended client program for the OpenVPN Access Server. The latest version of OpenVPN Connect client for macOS is available on our website.

Download OpenVPN Connect v3

sha256 signature: 4905f3088fedce5e75de46670735b616031aaa9eb22d1702289ac99d57e0f85f

For macOS versions titled El Capitan, Sierra, High Sierra, Mojave, Catalina, Big Sur, Monterey, and Ventura.

OpenVPN config file:

https://docs.truba.gov.tr/TRUBA/kullanici-el-kitabi/open-vpn/openvpn_info.html



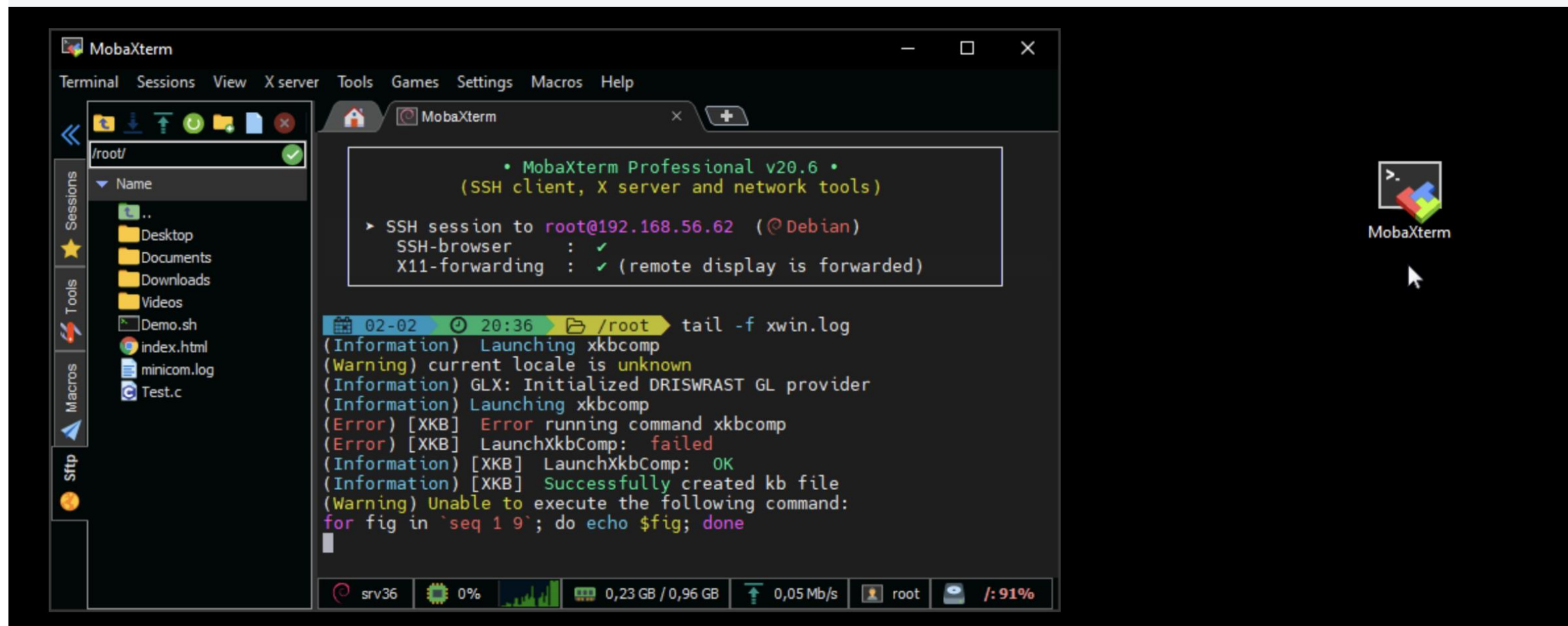
SSH Connection - Windows

Windows:

<https://mobaxterm.mobatek.net/>

MobaXterm

Enhanced terminal for Windows with X11 server, tabbed SSH client, network tools and much more



Dark mode: helps to reduce eye strain

 GET MOBAXTERM NOW!

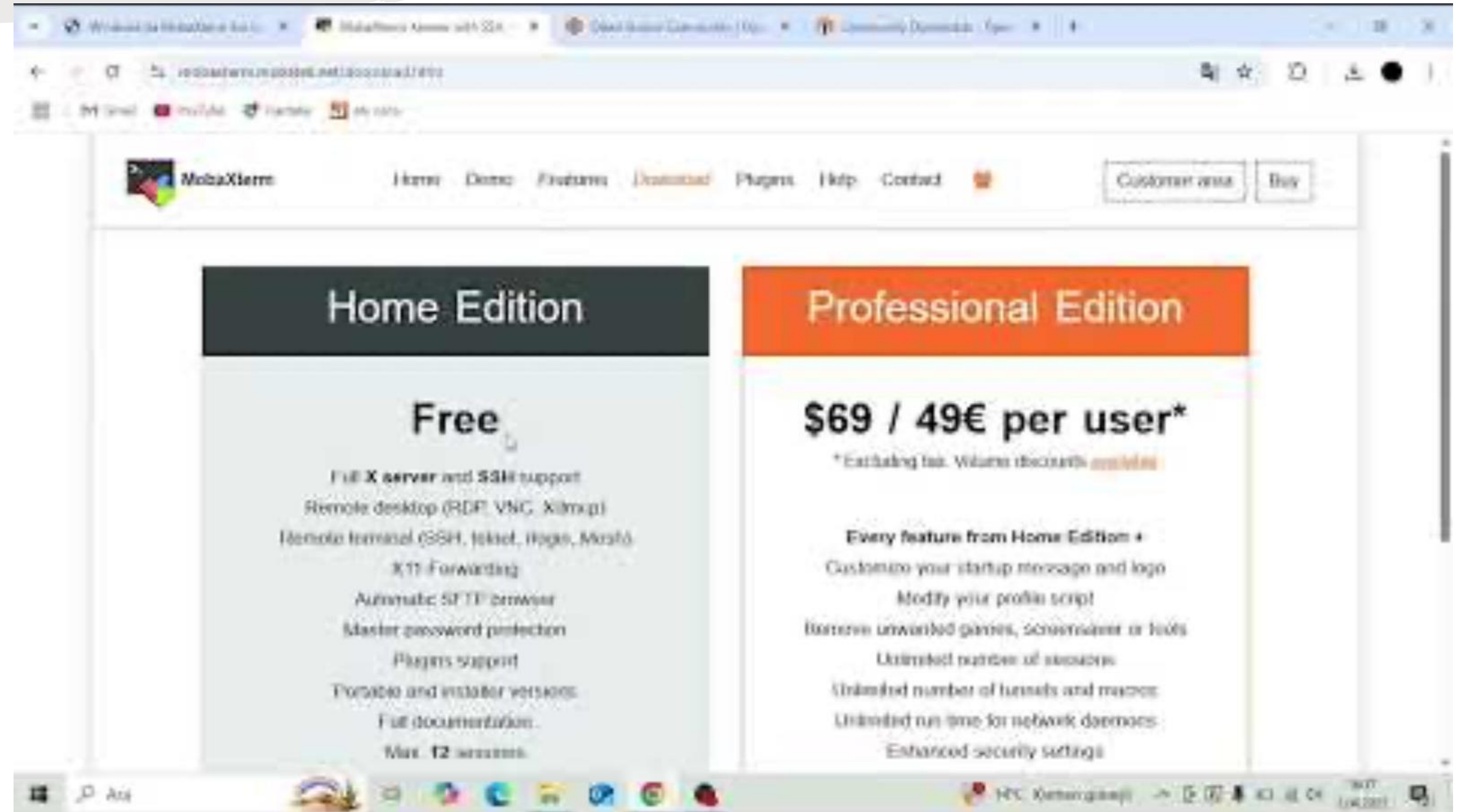
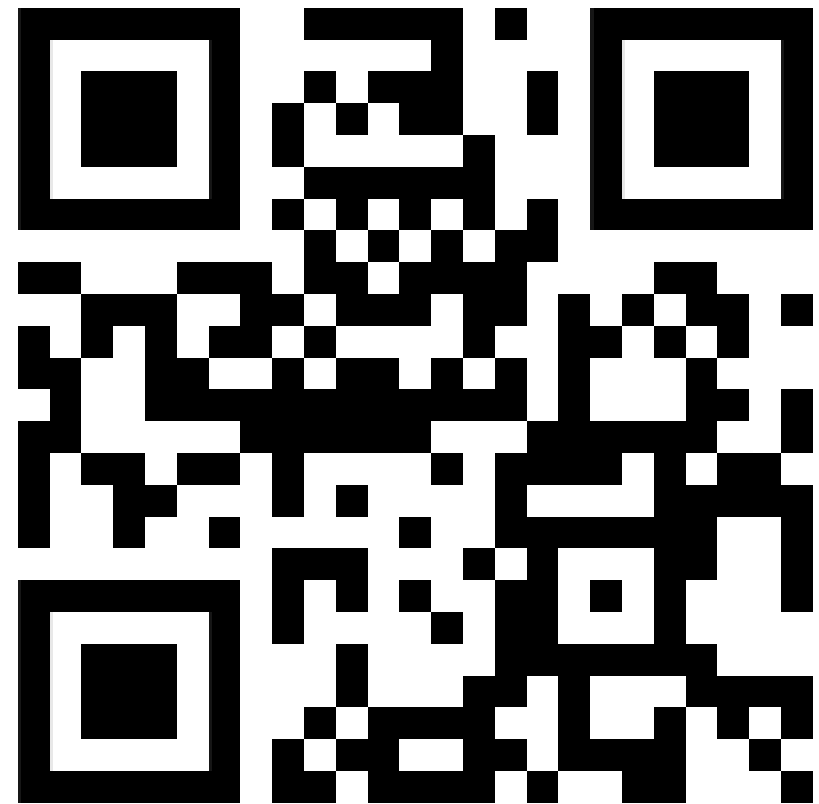


User Interface	Address
arf-ui1	172.16.6.11
arf-ui2	172.16.6.12
Open OnDemand	172.16.6.20
Grafana	172.16.6.25

```
ssh user_name@172.16.6.11
```

```
ssh -l user_name 172.16.6.11 (-l lower case 'L')
```

<https://youtu.be/nH1hpmLRrI0>



The screenshot shows the MobaXterm website with two pricing options:

Home Edition	Professional Edition
Free	\$69 / 49€ per user*
<ul style="list-style-type: none">Full X server and SSH supportRemote desktop (RDP, VNC, X11R6)Remote terminal (SSH, telnet, Rlogin, Ncrpc)X11 ForwardingAutomatic SFTP browserMaster password protectionPlugins supportPortable and installer versionsFull documentationMax. 12 screens	<ul style="list-style-type: none">* Excluding tax. Where discounts availableEvery feature from Home Edition +Customize your startup message and logoModify your profile scriptRemove unwanted games, screensaver or fontsUnlimited number of sessionsUnlimited number of tunnels and macrosUnlimited run time for network daemonsEnhanced security settings

- ❑ All jobs and resources in the cluster are managed by **SLURM**.
 - Your job scripts must include a section specifying your requirements for **SLURM**.
 - SLURM will schedule your jobs according to your requests and ensure they run as quickly as possible.
 - Script files (sample files: /arf/sw/scripts)
- ❑ When submitting your jobs to the queues, the following factors should be considered:
 - The number of cores and memory you will use
 - The expected runtime of your job
 - Selecting the correct queue based on the duration
 - Correctly specifying the runtime (in days-hours:minutes:seconds format)
 - The layout of your job (number of cores, number of servers, HyperThreading)
 - GPU usage
 - CPU usage



<https://slurm.schedmd.com/sbatch.html>

SLURM Script File

```
#!/bin/bash
#SBATCH -p debug
#SBATCH -A egitim
#SBATCH -J test
#SBATCH -N 1
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=4
#SBATCH -C weka
#SBATCH --reservation=bioexcel
#SBATCH --time=03:00:00

echo "SLURM_NODELIST $SLURM_NODELIST"
echo "NUMBER OF CORES $SLURM_NTASKS"

echo "number of CPUs= $SLURM_NPROCS"

module purge

module load apps/gromacs/2024.1-oneapi2024

#BURAYA is calistirma komutunuzu yaziniz

#mpirun gmx_mpi #Please add your gromacs commands

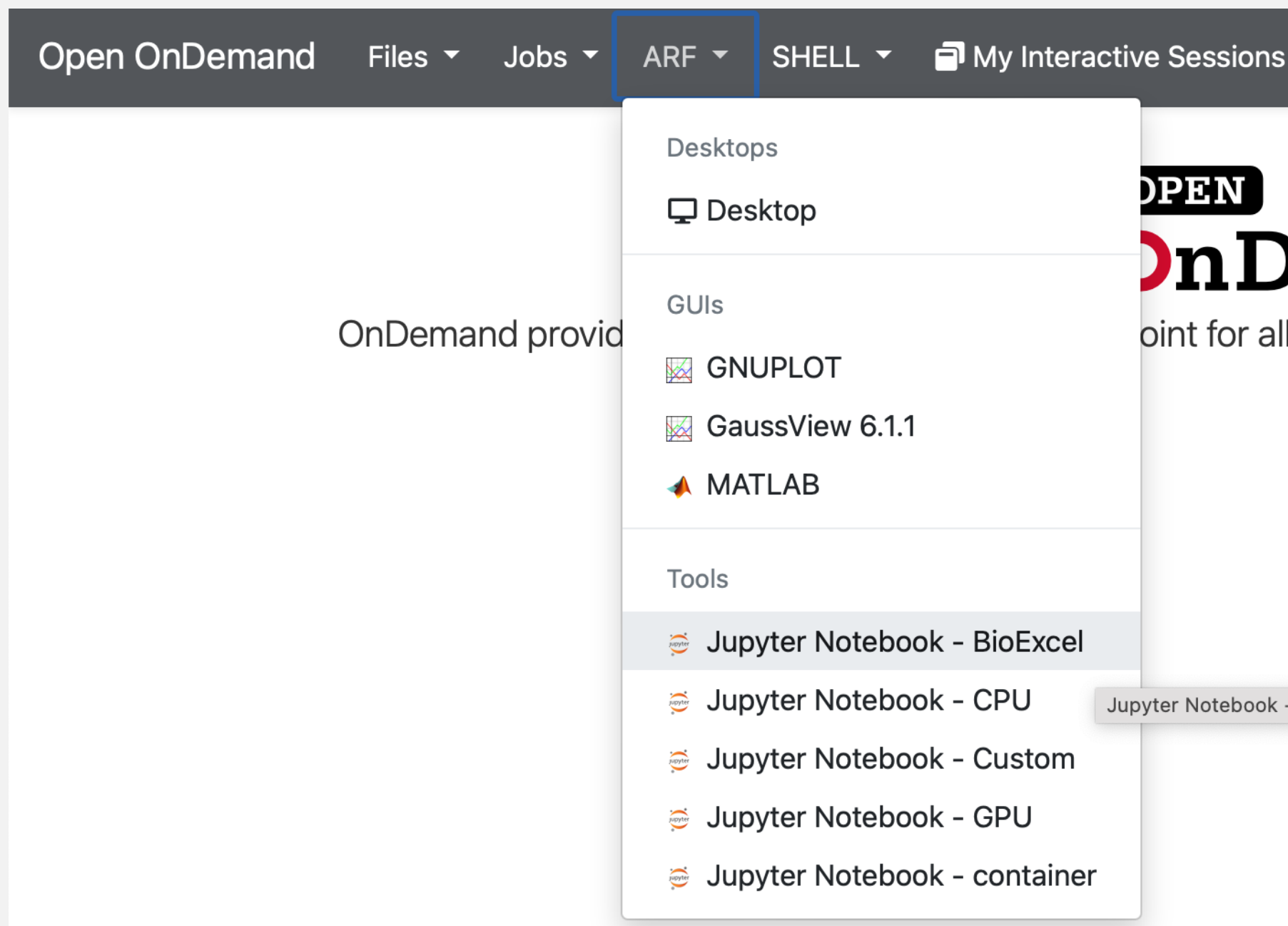
mpirun gmx_mpi mdrun -v -s benchmark.tpr

exit
```



benchmark.tpr	ener.edr	md.log	slurm-1056876.out	slurm-1944291.out	traj.trr
confout.gro	'#ener.edr.1#'	'#md.log.1#'	slurm-1056877.err	state.cpt	'#traj.trr.1#'
'#confout.gro.1#'	gromacs2024.1-oneapi2024-weka.slurm	slurm-1056876.err	slurm-1056877.out	state_prev.cpt	

- ❑ Open OnDemand service can be accessed with an internet browser at <https://172.16.6.20>
- ❑ Make sure your OpenVPN connection is active.



Jupyter Notebook - BioExcel

This app will launch a [Jupyter](#) Notebook server on one or more nodes. You may install Jupyter and other useful apps via [Anaconda](#). Please follow anaconda installation from [TRUBA-wiki].

Time limit (Hours)

Time limit for the job. Max 4 Hours

Launch

* The Jupyter Notebook - BioExcel session data for this session can be accessed under the [data root directory](#).



REPUBLIC OF TÜRKİYE
MINISTRY OF INDUSTRY
AND TECHNOLOGY

NATIONAL
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THANK YOU!

TÜBİTAK | THE SCIENTIFIC AND TECHNOLOGICAL RESEARCH INSTITUTION OF TÜRKİYE

User Support

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TRUBA HPC Center

<http://www.truba.gov.tr>

<http://docs.truba.gov.tr>

<http://portal.truba.gov.tr>

TRUBA Social Media

<https://www.linkedin.com/company/truba>



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