Report and plans on GPU accelerated HPCs in Hungary

Zoltan Kiss, KIFÜ
11-07-2019

Contents

- HPC in Hungary
  - About KIFÜ
  - Services
  - HPC Infrastructure
  - Statistics
  - Projects and collaboration
- HPC development
  - Infrastructure
  - Services
  - Collaboration
- Wrap Up
- Q&A

KIFÜ

KIFÜ

Serving the Hungarian Digital Transformation

HPC for research in Hungary

KIFÜ

User Community

- All **universities** and higher education institutes
- All academic **research institution**
- Nearly all the **public collections** (libraries, museums, archives)
- Primary and Secondary **education**
- **2.5 million** users are interacting with our services each day in more than 6000 institution

Non-HPC Services

- **Network**
  - Up to 100Gbps dedicated
- **Cloud**
  - IaaS Cloud based on OpenStack
    - 2880 vCPU, 9TB RAM, 2 PB storage
  - Webhosting
  - Web Drive
  - E-mail
- **AAI**
  - eduGAIN connected ID services
  - eduroam
- **Multimedia**
  - Video streaming portal, VoIP based TelCo service operator

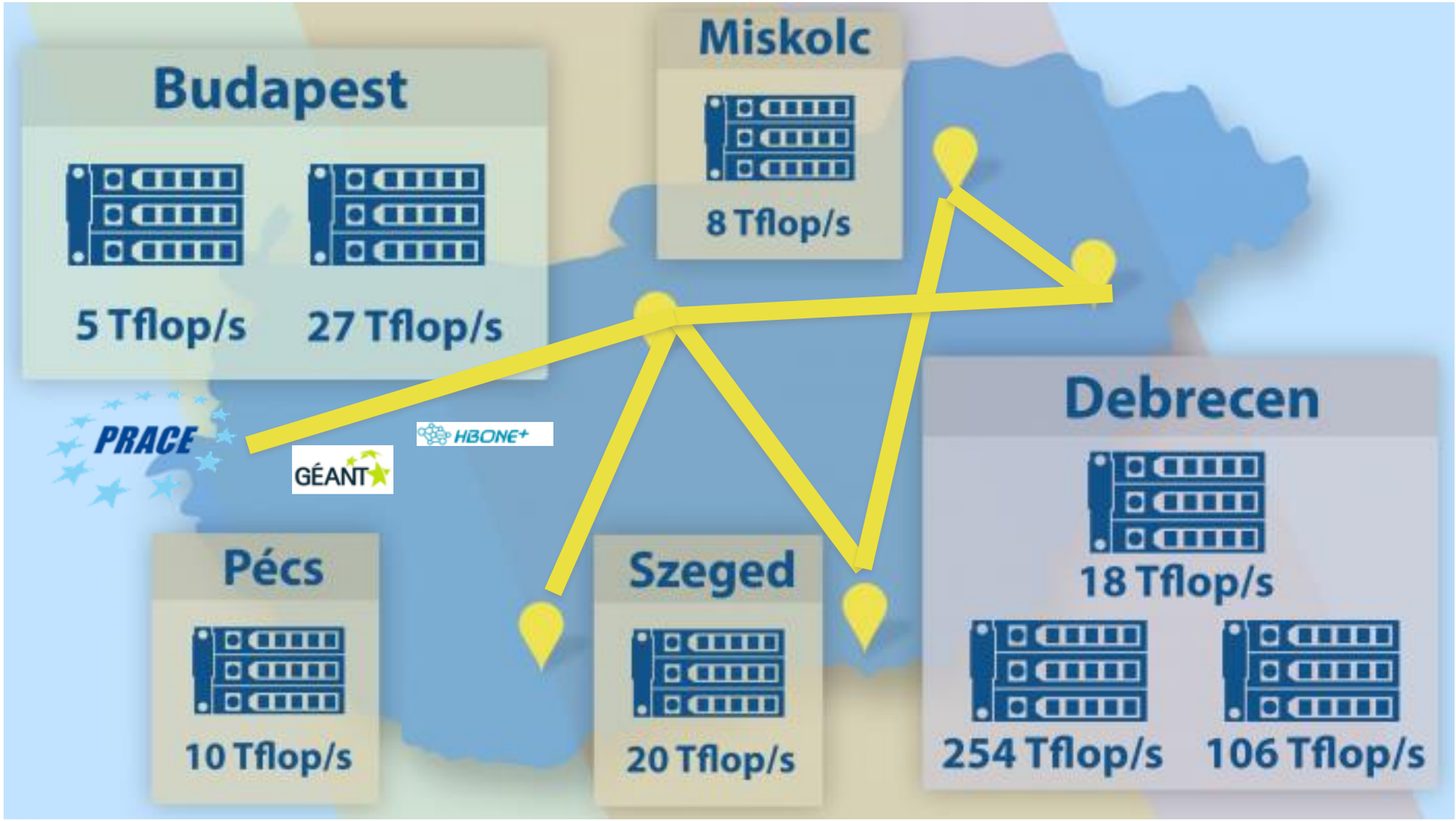
Why HPC?

- Central extreme capacity infrastructure to achieve fast results on high scale, designed for specific workloads
- National HPC capacity ~ competitiveness and R&D capabilities
  - Attract more researchers
- Lower cost / faster results
  - Virtualize labs
- Urgent computing
  - Tracking and forecasting current a future spread of fire, smoke, flood, plagues, etc.

Evolution of HPC

2001	2009	2011	2015	2021
60 Gflop/s	900 Gflop/s	48 Tflop/s	0.45 Pflop/s	15 Pflop/s

HPC Infrastructure



HPC Infrastructure

Location	Budapest2	LEO (DB2)	Apollo (DB3)	Miskolc
Type	HP SL250s	HP SL250s	HP Apollo 8000	SGI UV 2000
CPU / node	2	2	2	44
Core / CPU	10	8	8	8
Memory / node	63 GB	125 GB	128 GB	1.4 TB
Memory / core	3 GB	7.5 GB	8 GB	4 GB
CPU	Intel Xeon E5-2680 v2 @ 2.80GHz	Intel Xeon E5-2650 v2 @ 2.60GHz	Intel Xeon E5-2670	Intel Xeon E5-4627 v2 @ 3.33 GHz
GPU		68 * 3 Nvidia K20x + 16 * 3 Nvidia K40x		
Intel Xeon Phi	14 * 2 * Intel(R) Xeon Phi(TM) MIC SE10/7120		45 * 2 * Intel(R) Xeon Phi(TM) MIC SE10/7120	-
Linpack performance (Rmax)	27 Tflops	254 Tflops	106 Tflops	8 Tflops
Compute nodes	14	84	45	1
Dedicated storage	500 TB	585 TB	585 TB	240 TB
IC	IB FDR	IB FDR	IB FDR	Numalink 6

TOP 500 The List.

wiki.niif.hu/HPC_en

Debrecen HPC DC

Statistics

20 institution

70 Research field

381 project

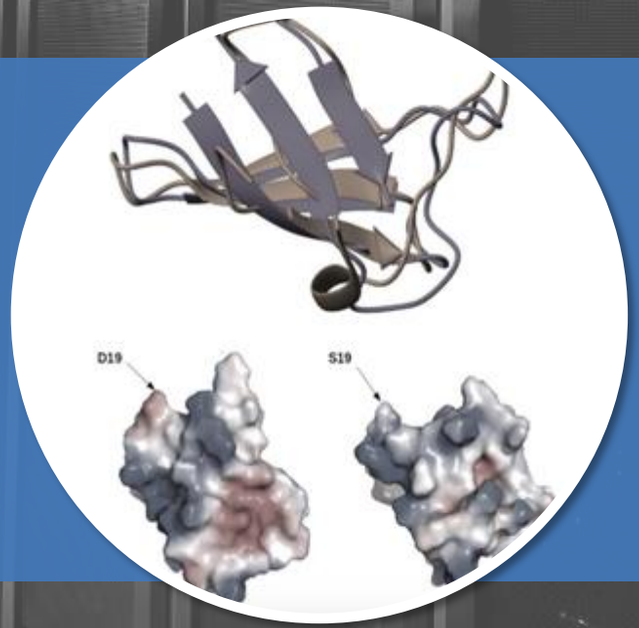
919 user

40M CPUh /year

>160 cumulated IF

7M Jobs

>43 publications*



KIFÜ HPC Portal

Bejelentkezve: Dr. Próba István (kilépés)

- Saját adatok
- Hírek
- Projektek
- Szolgáltatások állapota
- Hibabejelentés
- Grid Portal
- HPC Wiki

probaprojekt | nanographene | fluorinfra

Projekt információk

Teljes név:	HPC Portal Próba projekt 01
Projekt azonosító:	probaprojekt
Adminisztrátor felhasználók:	Dr. Próba István
CPU idő havi kvóta:	850 cpuh
Felhasznált CPU idő:	235 cpuh

Általános leírás:

Tanulmányunkban az önerősítéses polipropilén kompozit (SRPPC) lemezek ultrahangos hegesztéssel előállított átlapolt kötéseit vizsgáltuk, alapul véve a kompozit lemezek tulajdonságait...

Havi kvóta:

budapesti szupergép 01:	21.46%
debreceni szupergép 01:	60.32%
pécsi szupergép:	95.17%
szegedi szupergép:	13.81%

CPU idő igénylés | Projekt lezárás

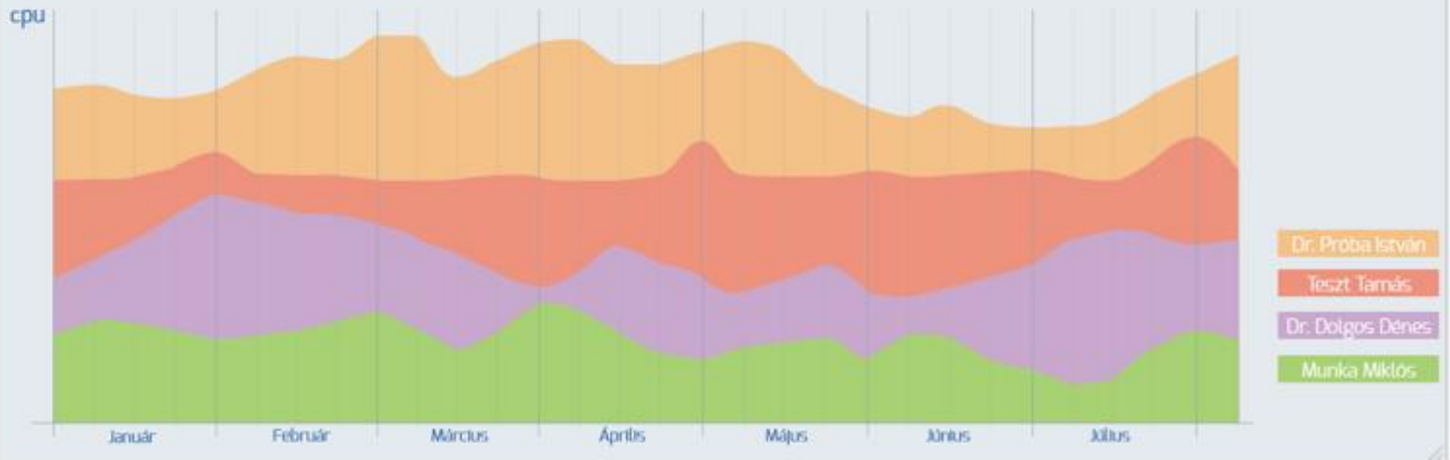
Felhasználók

Felhasználó név	Login név	Felhasznált CPU idő	Státusz
Dr. Próba István*	pp01-drproba	82 cpuh	admin
Teszt Tamás	pp01-tesztt	20 cpuh	aktív
Dr. Dolgos Dénes	pp01-drdenes	60 cpuh	passzív
Munka Miklós	pp01-munkam	12 cpuh	aktív

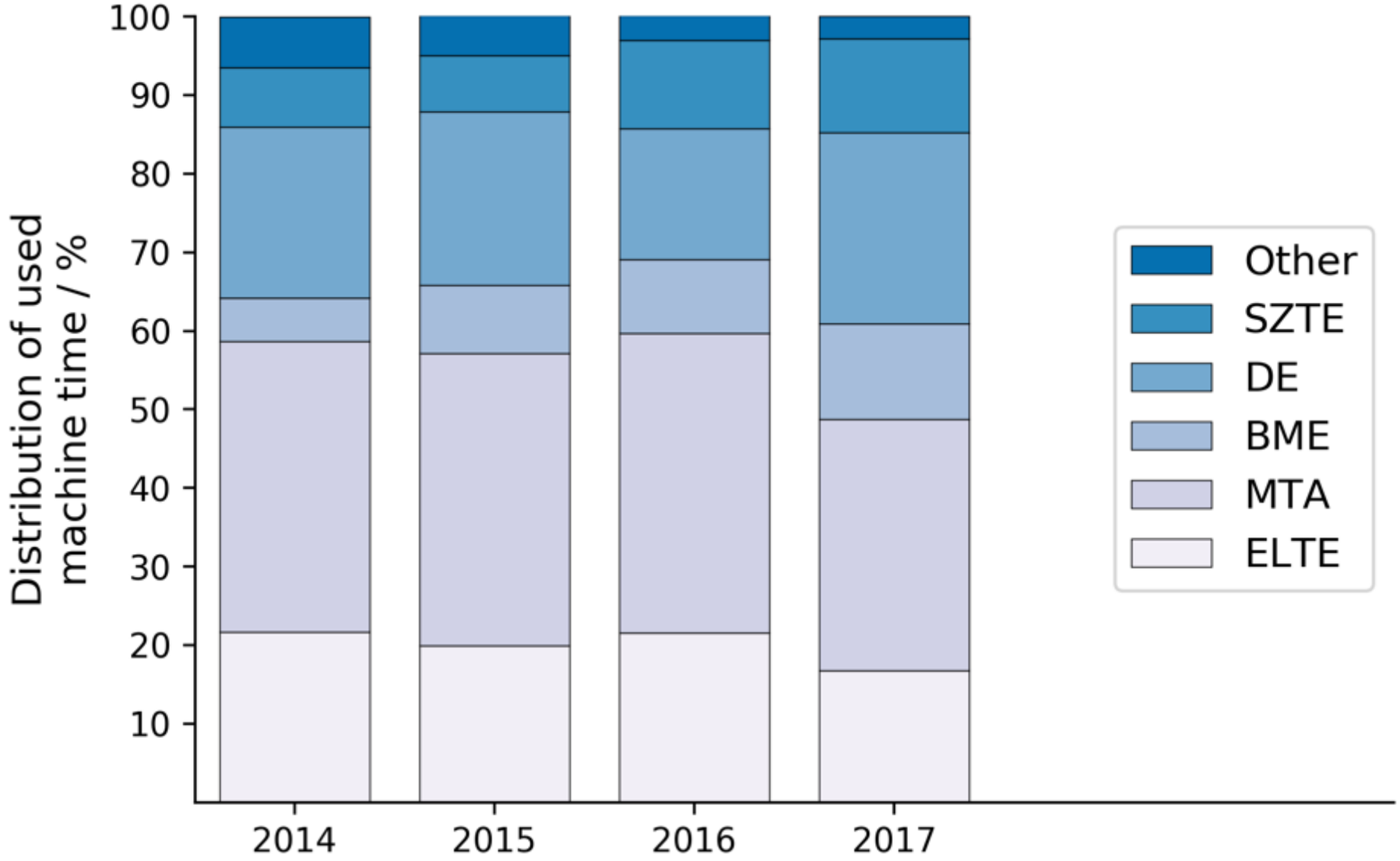
mintamarta@inviteduser.com — meghívó küldve: 2014.07.02 (2)
segitosandor@meghivott.hu — meghívó küldve: 2014.06.19 (1)

Meghívó küldése

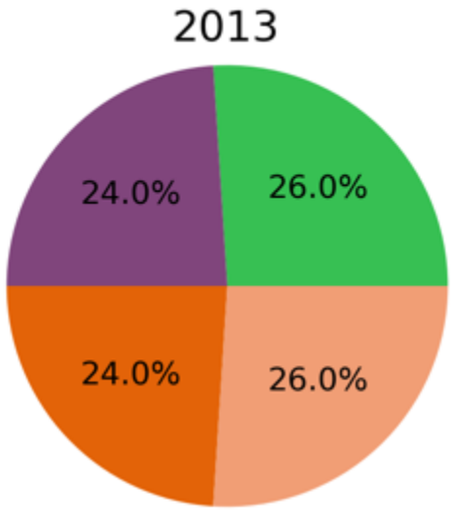
Statisztikai adatok

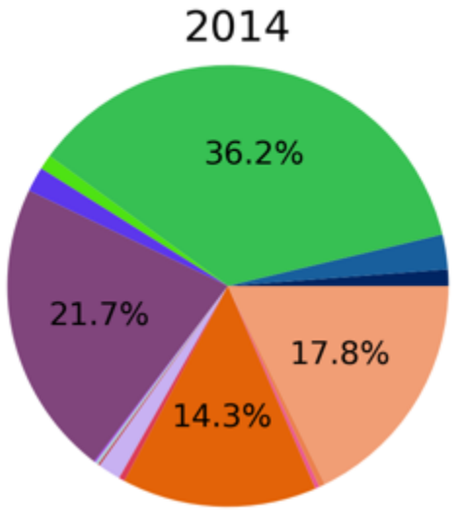


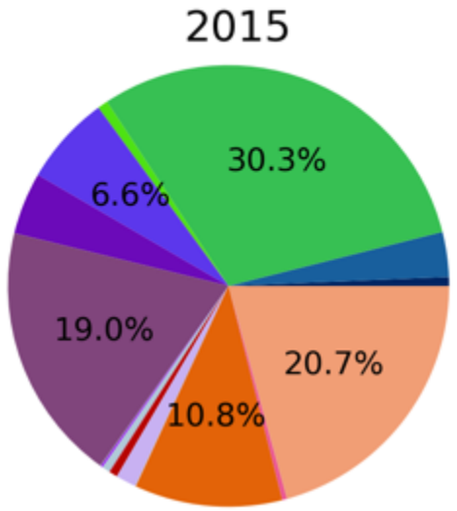
Top Institutions

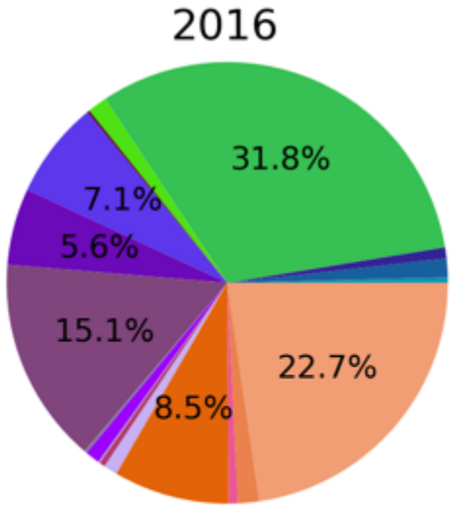


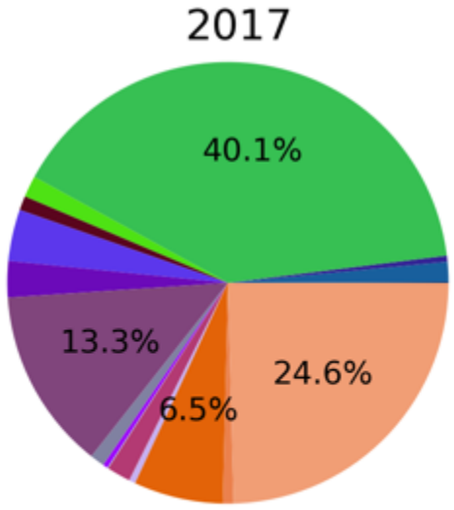
Research Fields











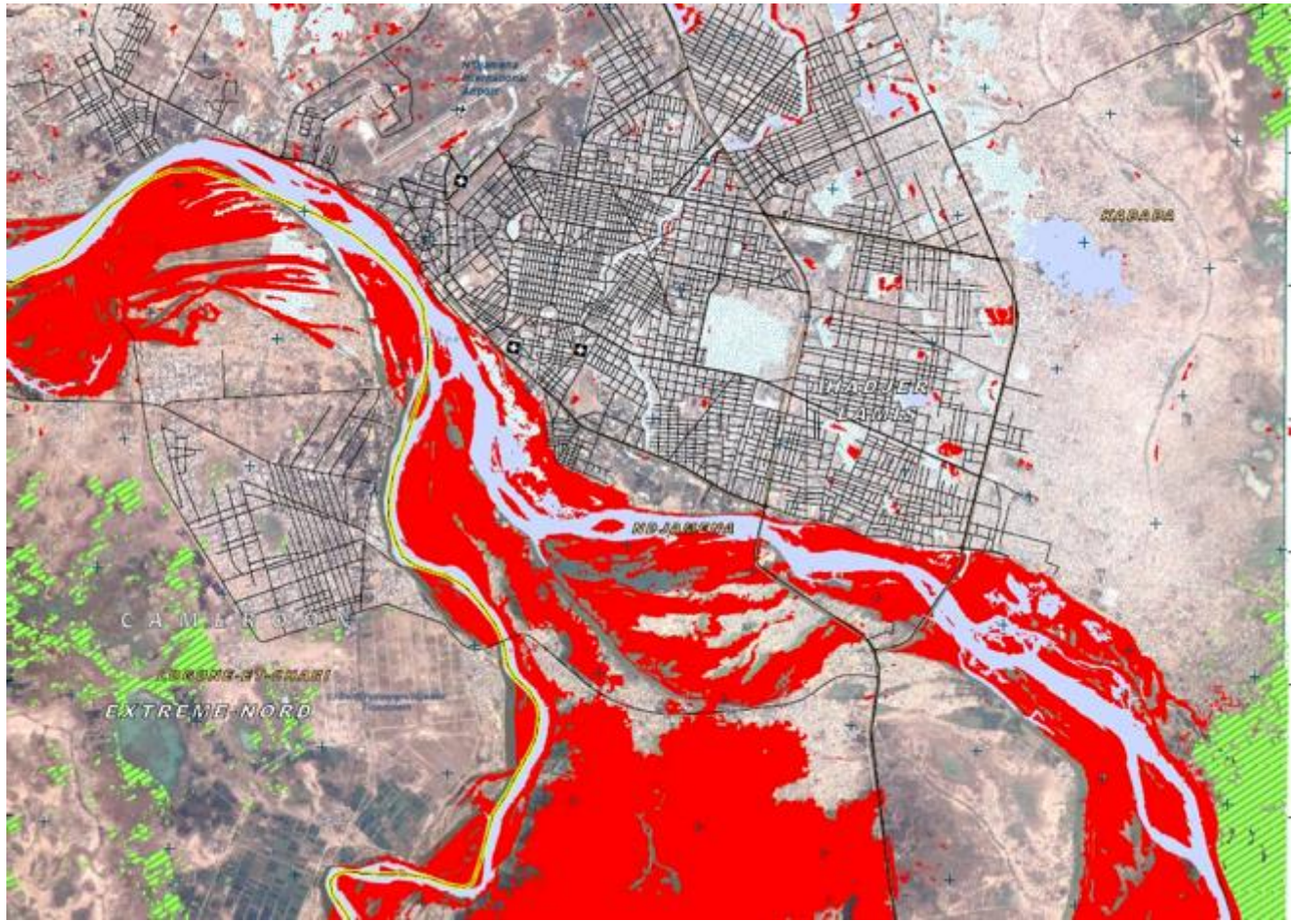
ELI-ALPS

- Extreme Light Infrasructure Attosecond Pulse Source
- Ultrashort impulses
- XUV, X-ray
- 4D imaging
- TW, PW intensity
- Analyze Electron movement

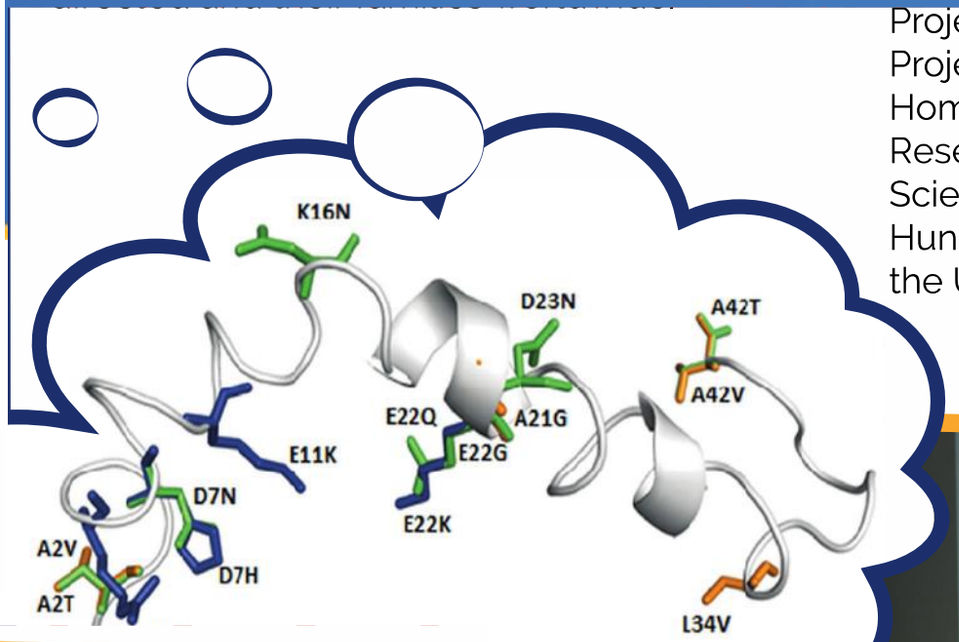
- Biological, Medical, IT, Industrial applications
- http://www.eli-hu.hu

Earth Information System Project

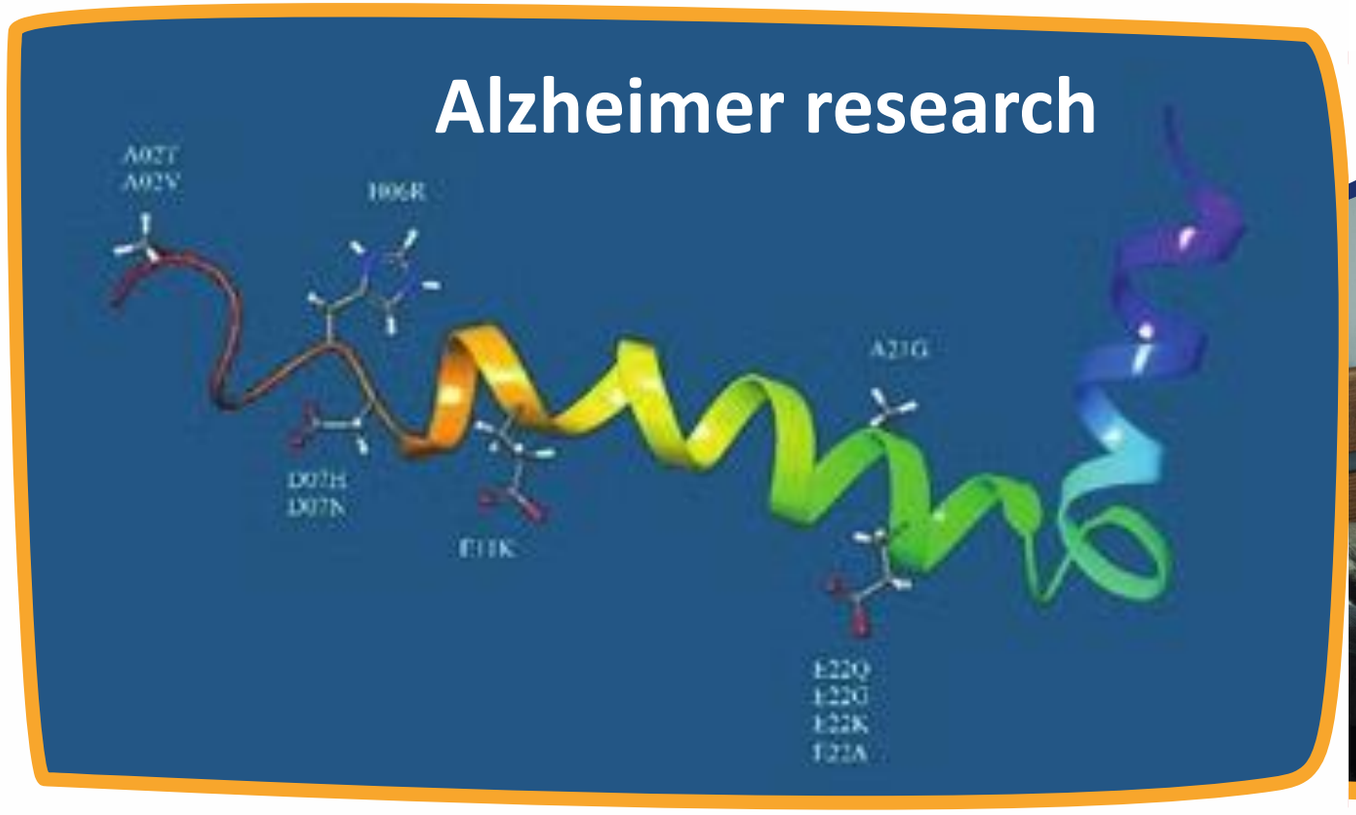
European Space Agency



The research group has been using Replica Exchange Molecular Dynamics (REMD) techniques, utilising the computational resources and power of the Debrecen2 (Leo) GPU cluster to analyse the molecular dynamics at play during this process. They have discovered connections between the presence of certain structures and mutated toxic peptides. This will hopefully increase the understanding, and ultimately the treatability of this disease, reducing the burden of suffering endured by those affected and their families worldwide.



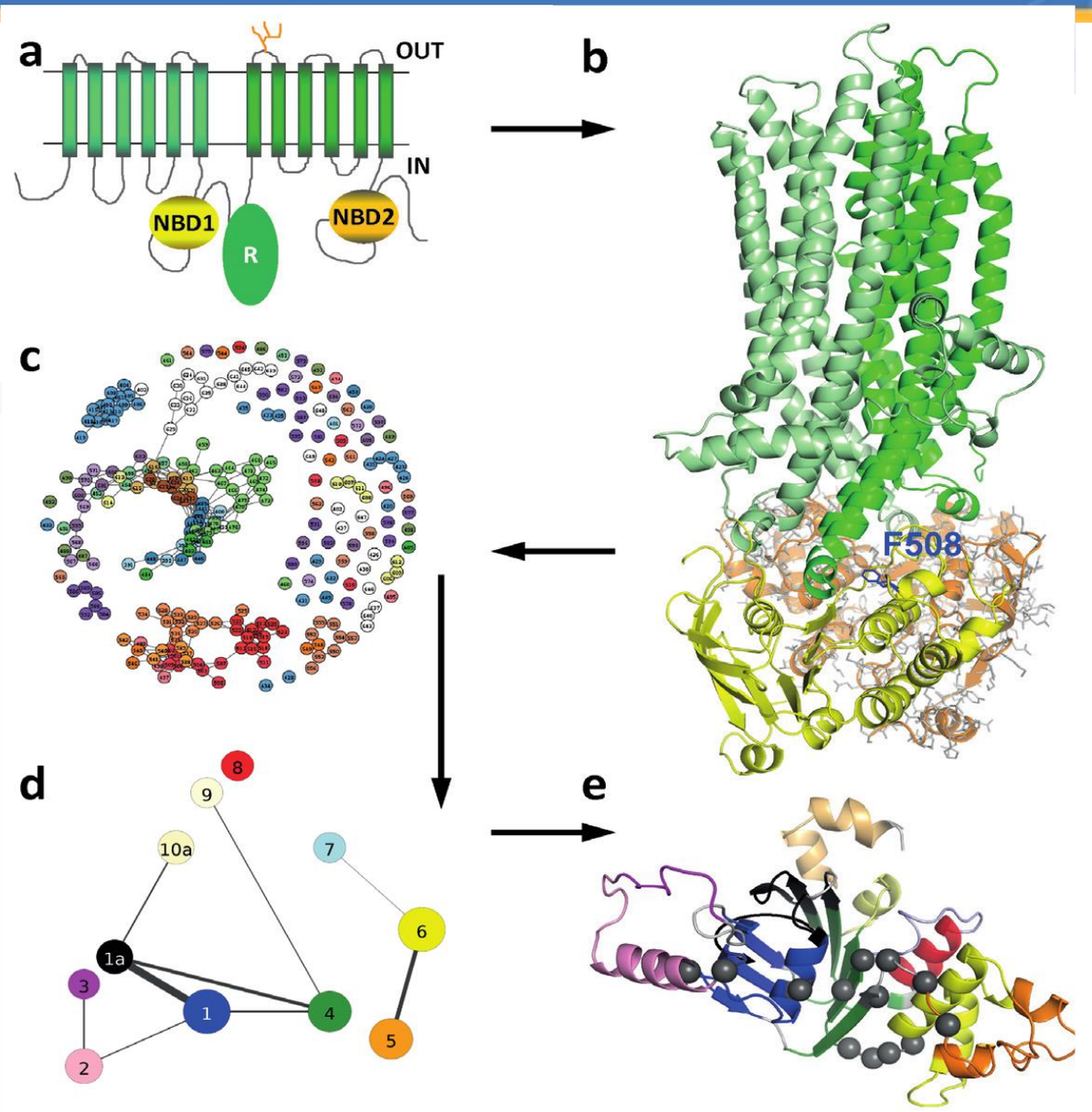
Project name: FEHERJEK
Project Leader: Gábor Paragi
Home inst.: MTA-SZTE Biomimetic Systems Research Group, the Hungarian Academy of Sciences – the University of Szeged, Szeged, Hungary, and the Institute of Physics, the University of Pecs, Pecs, Hungary



CFTR research potential cure to Cystic Fibrosys

The cystic fibrosis disease is caused by mutations in the gene of the CFTR protein, which is a chloride channel in the cell membrane.

objective in the field is to design drugs to restore the normal structural and dynamic properties of CFTR and deliver this channel to the cell

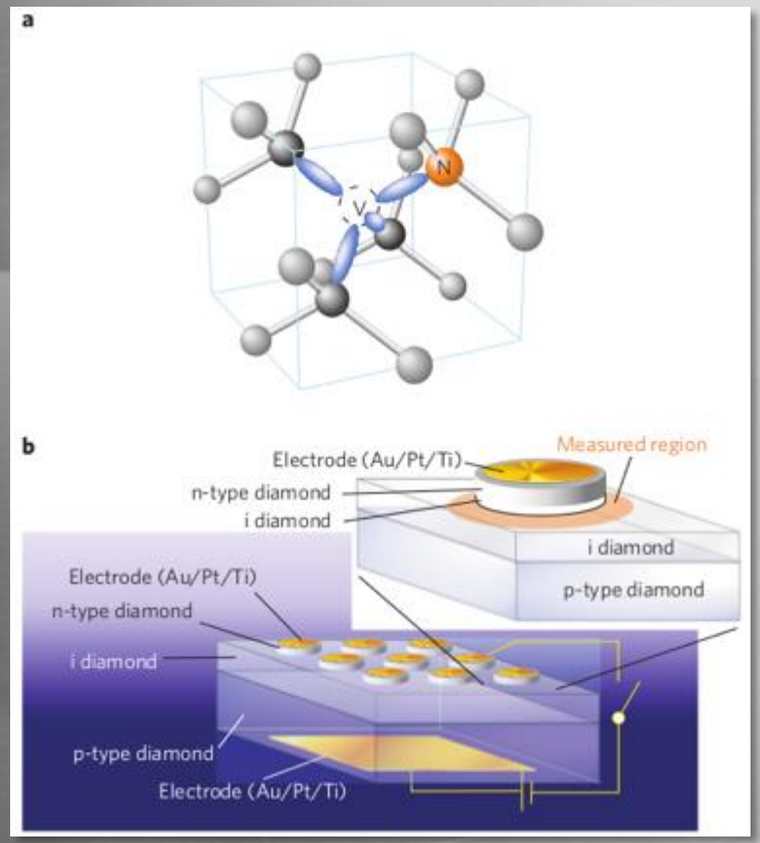


Project name: ABCFEH

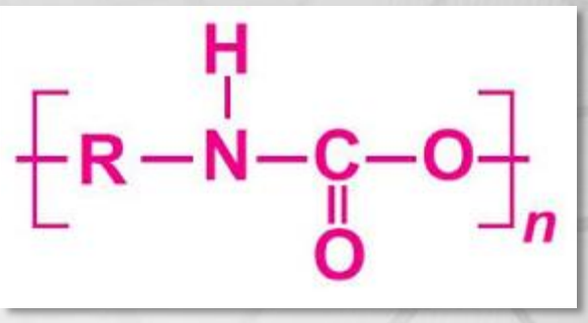
Project Leader: Tamás Hegedűs

MTA-SE Molecular Biophysics Research Group, the Hungarian Academy of Sciences, Budapest, Hungary and the Department of Biophysics and Radiation Biology, Semmelweis University, Budapest, Hungary

Industrial usage



BorsodChem
Chemistry for generations



RICHTER GEDEON

International collaborations

EuroHPC
Joint Undertaking

Interreg
Danube Transnational Programme
InnoHPC

GÉANT

elitrans

PRACE

Vi-SEEM

UP 2 U

4S

HPC Development Plans

HPC Development Plans

- Competitive hungarian HPC infrastructure as an important part of the european HPC ecosystem
- Domain or application specific support, HPC educational programme, Competence Center / DIH
- HPC community and ‚webshop-style' application portal for easy access, AI specific infrastructure, containers
- Raise awareness / Attract Research, SME and Industry

EuroHPC Joint Undertaking

HPC

Infrastructure development

- Maintain top100 position for entire lifecycle > 10Pflops system
- Low TCO
- Cluster + GPU preferred
- Centralized location
- Scalable infrastructure
- Drastically increase technical support team size along with scientific support
- Integration to the European HPC Infrastructure and Community

- Competitiveness
- Researchers

use non-eu machines

- 28 countries
- Exaflop
- 3 pre-exa, more peta
- IT + HU - pre-

Exa (150+ peta)

- 1M+ EUR for R+I

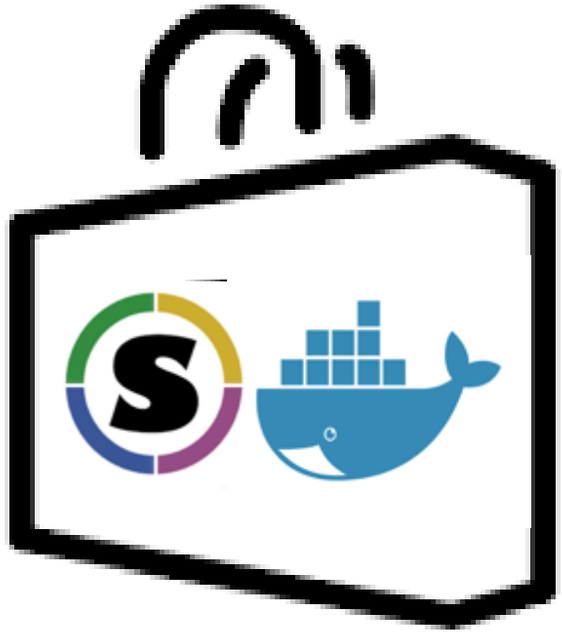
Sign up for calls

HPC Competence Center

- Create domain specific support network of experts (at least 12 FTE)
- Collaborating with Tier-2/3 level research centres
- Provide effective training portfolio offered to group of users
- Effective domain or application specific support
- Programme to involve SME / Industry
- Interact with international (e.g. exascale) centres
- Act as / interact with Digital Innovation Hub(s)
- Joined EuroHPC with

Application related developments

- HPC + Cloud integrated ’Application Webshop’
  - Short life fully customized applications
  - Container support
  - Orchestrator
  - Platform + Licence as a service

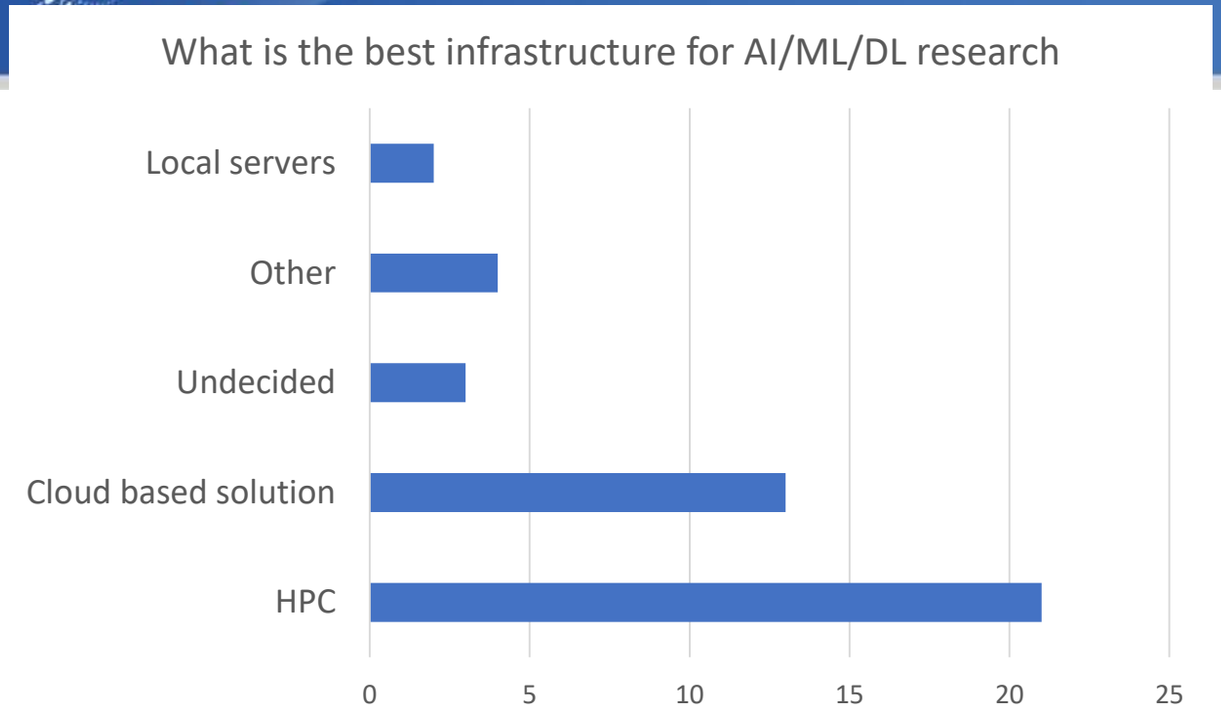


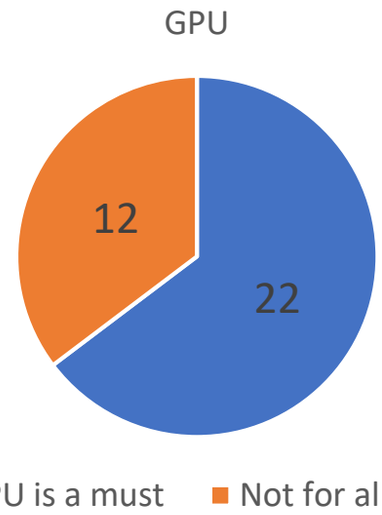
- Big Data + AI + Blockchain
  - Integration with multi tier storage onsite: iSCSI, HSM, Tape
  - BD + AI / specific hardware / applications

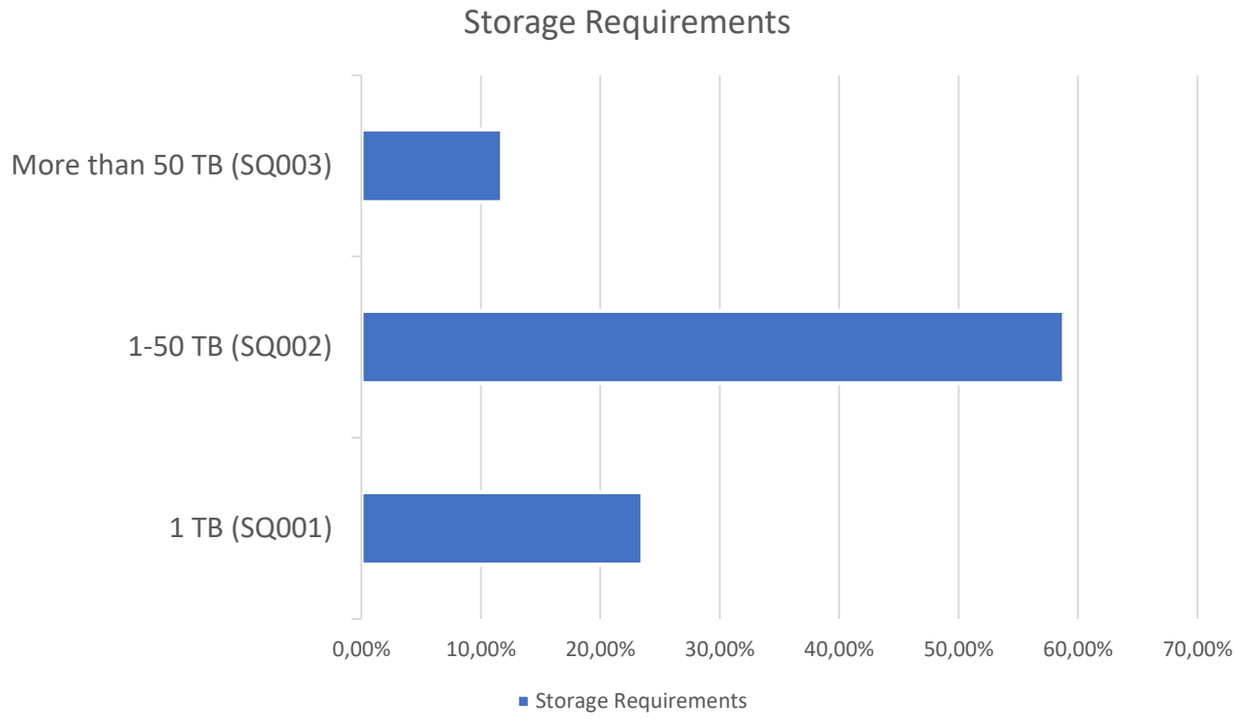
- Workflow managment support

AI

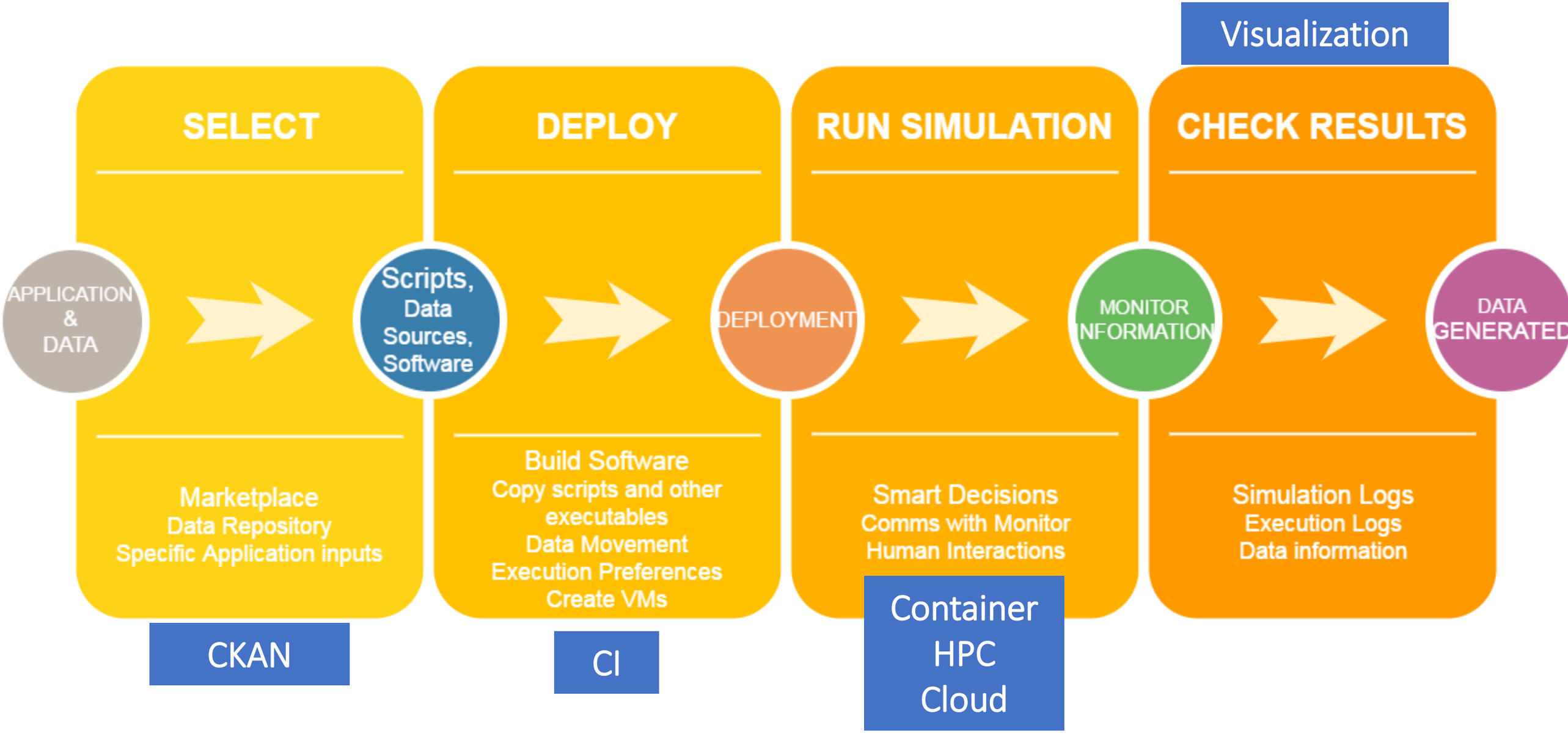
AI / ML survey


What is the best infrastructure for AI/ML/DL research
Local servers
Other
Undecided
Cloud based solution
HPC
0
5
10
15
20
25


GPU
12
22
GPU is a must
Not for all cases


Storage Requirements
More than 50 TB (SQ003)
1-50 TB (SQ002)
1 TB (SQ001)
0,00%
10,00%
20,00%
30,00%
40,00%
50,00%
60,00%
70,00%
Storage Requirements

HPC Portal workflow - example



Wrap Up

- KIFÜ is effective ICT Infrastructure operator and developer with at least 30 years of experience, and has 18 years of history operating HPC
- The Agency has been in International e-Infrastructure technology development collaborations and projects since 2000 as a primary source of adopting new technologies into production
- We are constantly working on to offer the most advanced, but cost effective ICT services for research and development.

Q&A

www.kifu.gov.hu

hpc.niif.hu

Zoltan Kiss
Head of Information Systems Department
kiss.zoltan@kifu.gov.hu

11th July, 2019