COMPUTE SERVICES/METACENTRUM

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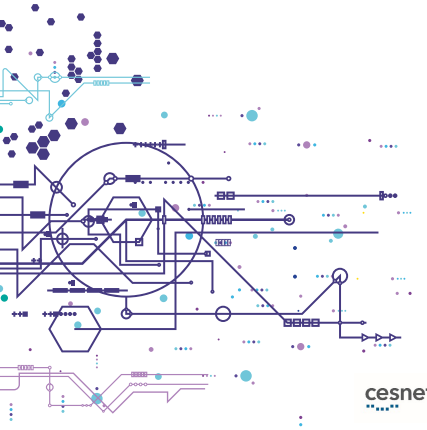
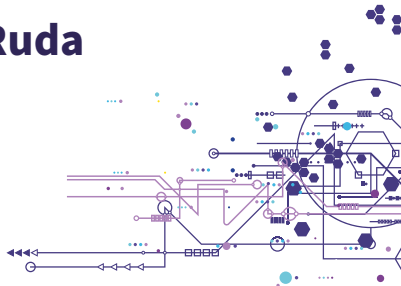
November 2022

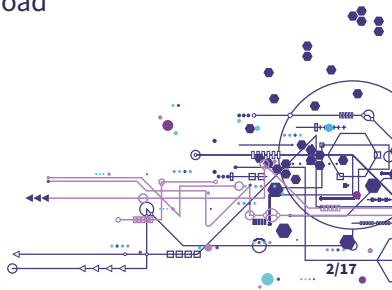




MetaCentrum I

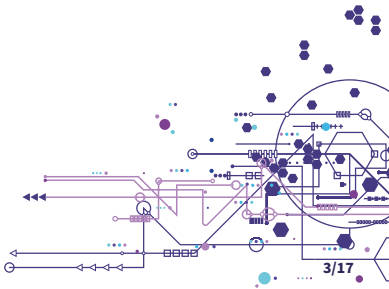
National distributed computing environment, CESNET coord.

- resources both by CESNET and CERIT-SC (50.000 CPU cores)
- compute resources located at CESNET, universities, CAS
  - original motivation of resource sharing (HW) still valid
  - providing temporarily free resources for remote users
  - usage of remote resources in case of urgent/heavy load
  - and use other resources during an outage
  - resources for project start-up, HW suitability check
  - idea works also for expensive commercial licenses
- community access, central management and AAI
- grid, cloud and map-reduce computing models
- virtualization platform for highly available services



MetaCentrum II

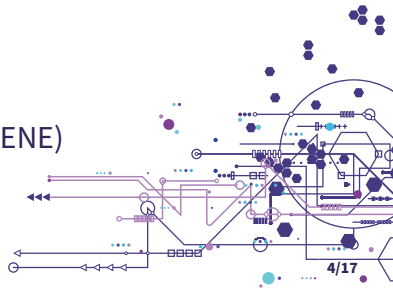
- distributed model useful for different use-cases
  - integration of resources owned by other RIs (ELIXIR)
  - big-data use-cases - no need for remote transfer
  - architecture compatible with distributed data repositories in EOSC CZ NDI
- NGI in European e-infrastructure EGI, EOSC mandated org.
- targeted support for large projects (VI, ESFRI)
- umbrella for development of new services/tools
  - OnDemand, Jupyter, Galaxy, Kubernetes
  - support for processing of sensitive data
- (very) similar technology with IT4Innovations
  - further unification in e-INFRA CZ



Cooperation with partners

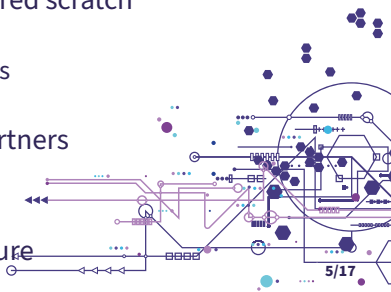
Collaboration with projects = motivation to develop new services

- LHC, Auger, CTA, Belle
  - original motivation of the grid, still active in EGI
- ELIXIR (OpenScreen, CCT, Czech Bioimaging)
  - collaborating VIs, resources integrated into MetaCentrum
  - cooperation in the operation of ELIXIR services
  - life-science is the largest consumer of resources
- ELI, BBMRI, LINDAT/CLARIN, ICOS
  - especially at international/project/EGI level
- research centres CzechGlobe, CEITEC, (Recetox, EIRENE)
  - long term users, link through CERIT-SC (MU)
- ESA – CollGS, Data Relay Hub
  - various groups/project using Coppernicus data



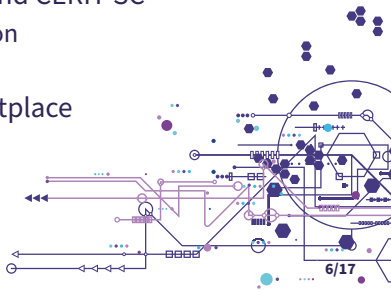
MetaCentrum computational models I

- grid, centrally managed HTC, HPC clusters
  - batch, long (dayes/weeks) jobs
  - both HTC and parallel computing (PBSPro)
  - including interactive tasks, GUI
    - Galaxy, Jupyter, OnDemand
  - semi-permanent storage (GPFS+NFS) and local/shared scratch
  - computations also in containers (Singularity)
    - HPC approach, support for non-root Docker images
    - NVIDIA GPU Cloud software
  - distributed clusters of e-INFRA CZ members and partners
    - development and research in area of scheduling
    - origins of Perun development (AAI)
  - subset of resources available also in EGI infrastructure



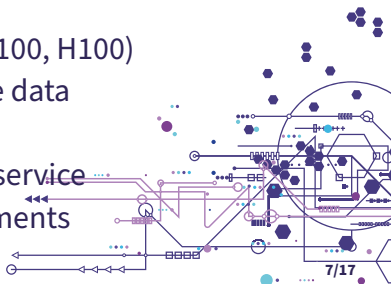
MetaCentrum computational models II

- MetaCentrum cloud - virtual machine instead of tasks
  - images provided by MetaCentrum, EGI, projects, users
  - cloud computing and services for computing (OpenStack)
    - but also training, teaching, KYPO security polygon
  - Terraform or EGI Infrastructure Manager for virtual clusters/K8s
  - central installation in Brno, joint effort of CESNET and CERIT-SC
    - in 2022 development of new OpenStack distribution
    - plan for second installation in IT4I in 2022/2023
  - site access also through EGI FedCloud, EOSC Marketplace
- MapReduce - Hadoop/Spark, data processing
  - dedicated cluster replaced by cloud images

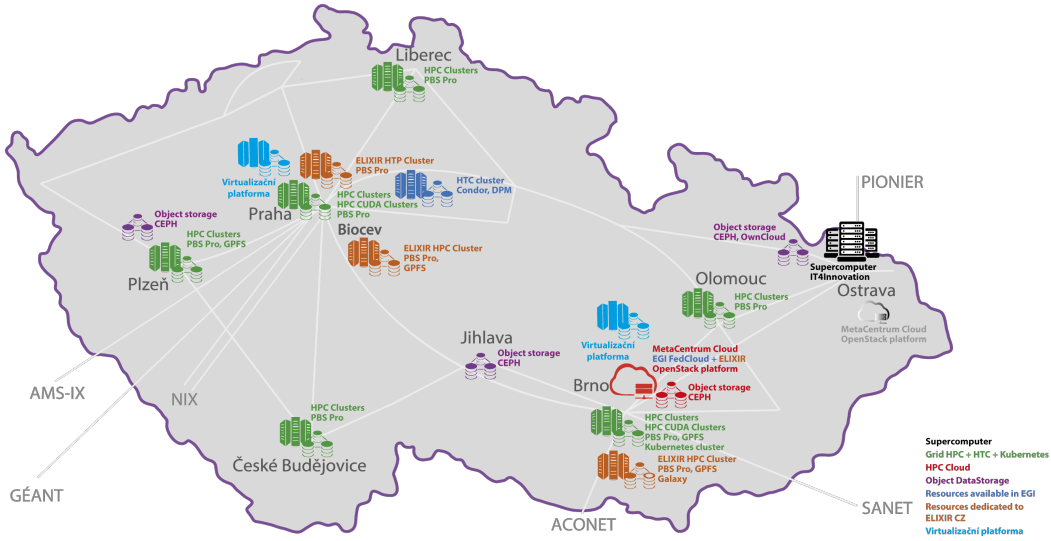


MetaCentrum computational models III

- containerized cloud
  - Kubernetes for micro-services, managing virtual environments
  - managed service, non-root containers, Rancher GUI
  - strong support for interactive and workflow requirements
    - SaaS approach for Matlab, RStudio, NextFlow
  - development in area of converged computing
    - integration of batch system and Kubernetes
- NVIDIA GPU cards available in all platforms (up to A100, H100)
- work on use-cases related to processing of sensitive data
  - currently Kubernetes, later also OpenStack
- we are also responsible for EGI Jupyter and Binder service
- virtualization platform for services with HA requirements
  - VMWare, two sites in Brno and Prague

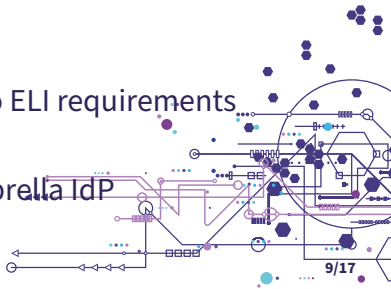


Architecture of MetaCentrum



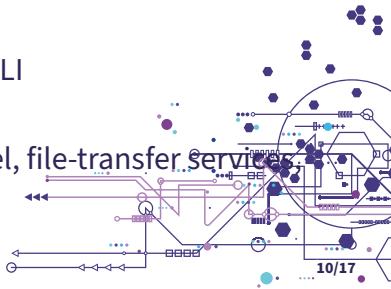
Collaboration opportunities with ELI I

- integration of ELI computing resources into MetaCentrum
  - central management, shared installations of application software
- design of a joint installation of resources at the ELI site
  - unified architecture of deployment ELI and CESNET resources
  - fast access to data resources of all partners (ELI, MetaCentrum, CESNET S3 storage)
  - see example of such approach in Biocev
- development of MetaCentrum services according to ELI requirements
  - JupyterHub, Galaxy, OpenStack, Kubernetes
- cooperation in the area of use/development of Umbrella IdP



Collaboration opportunities with ELI II

- joint development and operation of services developed in the PaNOSC project
  - Jupyter, VISA portal
  - tools towards FAIR data
- collaboration within the thematic repository in EOSC CZ
  - see afternoon presentations for details
- possible help with installation of cloud services in ELI
  - on ELI resources (Openstack, Kubernetes)
- other possible topics – Science DMZ at network level, file-transfer service, secure virtualization platform

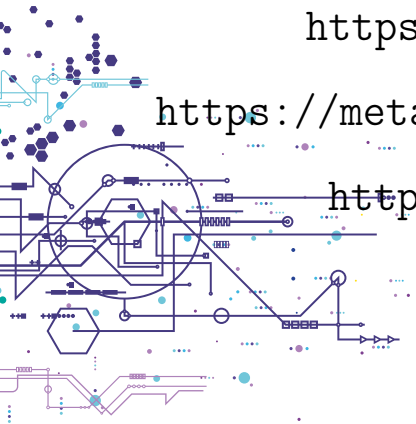


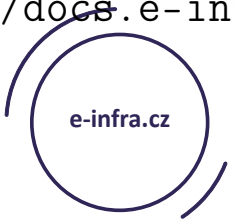
Thanks for your attention

https://www.metacentrum.cz

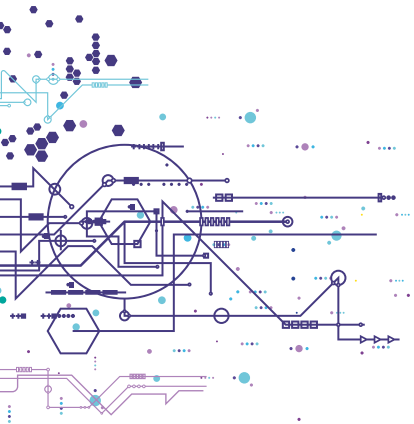
https://metavo.metacentrum.cz/en/state/

https://docs.e-infra.cz/

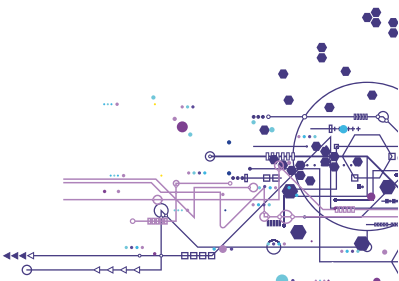




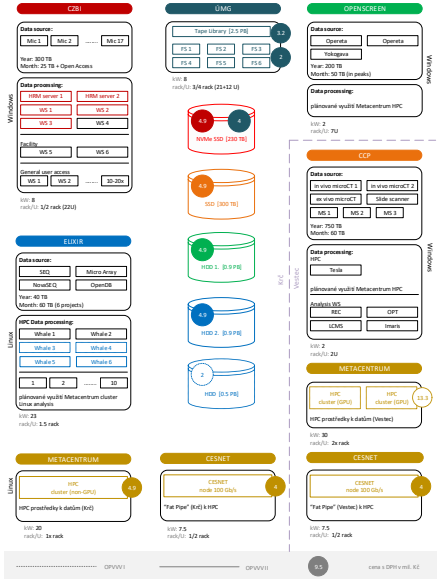
Backup slides



e-infra.cz



HPC datová infrastruktura ÚMG



Long-term development

	2012	2014	2016	2017	2018	2019	2020	2021	10-2022
Počet uživatelů MC	613	1112	1611	1908	2020	2185	2225	2606	**2523**
Noví uživatelé (Meta)	312	605	742	732	713	762	774	792	**771**
Počet úloh [milion úloh] Meta/EGI	1,1/ n/a	3,9/ n/a	3,6/ 6	4,7/ 7	5/ 6,7	8,6/ 6,8	13,1/ 10	12,1/ 9,3	**9,9** jen grid
CPU čas [CPU let] Meta/EGI	2500/ n/a	6403/ n/a	9475/ 5963	10572/4 622	11357/40 74	13129/45 31	16630/9 160	22647/ 9581	**16548** grid, K8s
Počet CPU jader vč. EGI	6028	14164	17234	18666	21344	26602	29874	34084	**37994** CESNET + 3264 CERIT + 1152 NCBR - 940
Počet GPU						255	322	434	**520** -NCBR

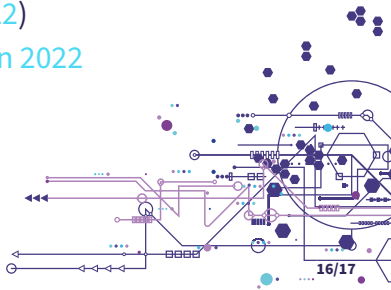
Cluster usage 2021

MetaCentrum 2021	Celkem MetaV0	meta-pbs	cerit-pbs	elixir-pbs	MetaCentrum Cloud	Kubernetes
Počet úloh / spuštěných VM strojů (2021)	**12 172 476**	6 575 865	4 638 124	943 360	15 127	v provozu od října 2021 n/a
Propočítaný CPU čas (walltime) [CPU let] (2021)	**22 647**	11558	4615	1621	4481 (včetně 641 FedCloud)	373
Počet uživatelů ke konci prosince 2021	**2606** uživatelů MetaVO			**86** uživatelů ELIXIR-CZ VO	**176** projektů / **535** individuálních účtů	10 projektových účtů
Alokovaná kapacita CPU jader prosinec 2021	**34 084**	**17164** z toho CESNET 10972	**6656** (6384 CERIT, 112 UEB, 160 elixir)	**2936** (plus 160 eli v pbs-cerit)	**6048** (MUNI, CESNET, CERIT-SC, ELIXIR-CZ,…) **+ 3424** export pbs-cerit	**1280** (2560 HT jader)
Počet evidovaných GPU karet ke konci prosince 2021	**434**	**288**	**20 + 40** z cloudu	**0**	**52 + 40** export do PBS	**34**
Alokovaná kapacita CPU jader duben 2022	**38 884**	**20428** z toho CESNET 14236	**6656** (6384 CERIT, 112 UEB, 160 elixir)	**2936** (plus 160 eli v pbs-cerit)	**6176** (MUNI, CESNET, CERIT-SC, ELIXIR-CZ,…) **+ 3424** export pbs-cerit	**1344** CERIT-SC (2668 s HT)
Počet evidovaných GPU karet v dubnu 2022	**531**	**368**	**20 + 40** z cloudu	**0**	**63 + 40** export do PBS	**40**
Storage konec 2021	obsazeno **7,6 PB** z celkových **15 PB**			obsazeno **600 TB** z **2 PB**, z toho 1,7 PB pro citlivá data	obsazeno **200 TB** z celkových **1,4 PB**	n/a
Publikace s poděkováním MC/NGI z 2021	**381 Perun / 414 WoS**					

https://metavo.metacentrum.cz/cs/state/stats/2021/

HW resources – 2022

- end of 2022: 50.000 CPU cores (x86_64)
  - HD nodes - 32-128 CPU cores, 256-1024 GB RAM
  - SMP servers - 2-3 TB RAM
    - specialized servers with 6/10 TB RAM
  - GP-GPU cards - 141+40 nodes, 380+110 cards
    - NVIDIA T4, 1080 Ti, 2080 Ti, A100, A40, H100
- CESNET (23.000, of which an increase of 6144 in 2022)
- CERIT-SC (8.000 CPU cores, DGX-2 with H100 cards in 2022
- clusters provided by other partners
  - VI ELIXIR (5824)
  - FZU (5190 for LHC/EGI)
  - ZČU, MU, UK, TUL, AV ČR, ~~CEITEC~~ (-912 in 2022)
- 15 PB disk storage for semi-permanent data



GPU cards in MetaCentrum

- CESNET cluster `adan`, 122x NVIDIA T4, <- main HTC resource
- CESNET cluster `galdor`, 88x NVIDIA A40 <- HPC cluster
- CERIT `glados`, 35xNVIDIA 1080Ti (15 in cloud)
- CERIT cluster `gita`, 28x 2080 Ti (16 in cloud)
- CERIT cluster `zia`, 20x NVIDIA A100 <- most powerfull card
- clusters of partners KKY ZCU, NATUR UK
  - server `cha.natur.cuni.cz`, 8x GeForce 2080 Ti
  - cluster `fau.natur.cuni.cz`, 8x Quadro RTX 5000
  - cluster `fer.natur.cuni.cz`, 32x RTX A4000 <-2022
  - cluster `konos`, 32x GeForce 1080Ti
- OpenStack cloud
  - 20xNVIDIA T4 CESNET, 12xNVIDIA T4 ELIXIR
- Kubernetes CERIT-SC, 24xNVIDIA A40, 6xNVIDIA A10,
  - 12xNVIDIA A100, 2xNVIDIA H100 <-2022