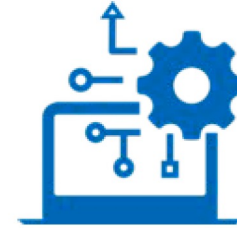




DIRAC EGI service

*A. Tsaregorodtsev
CPPM-IN2P3-CNRS, France,
DIRAC User's Workshop, 19 June 2024,
CC/IN2P3, Doua, France*

- ▶ EGI Workload Manager – official service in the EGI portfolio
- ▶ Service hosting at CC/IN2P3
 - ▶ Openstack VMs
 - ▶ 2 development servers
 - ▶ DIRAC v9.0.0a29
 - ▶ 1 Alma Linux VM for the DIRAC certification tests
 - ▶ MariaDB server
 - ▶ Elasticsearch server
- ▶ 1 server at CPPM, Marseille
 - ▶ CS, SE
- ▶ DIRAC 8.0.24
 - ▶ DIPS services
 - ▶ Tornado TokenManager



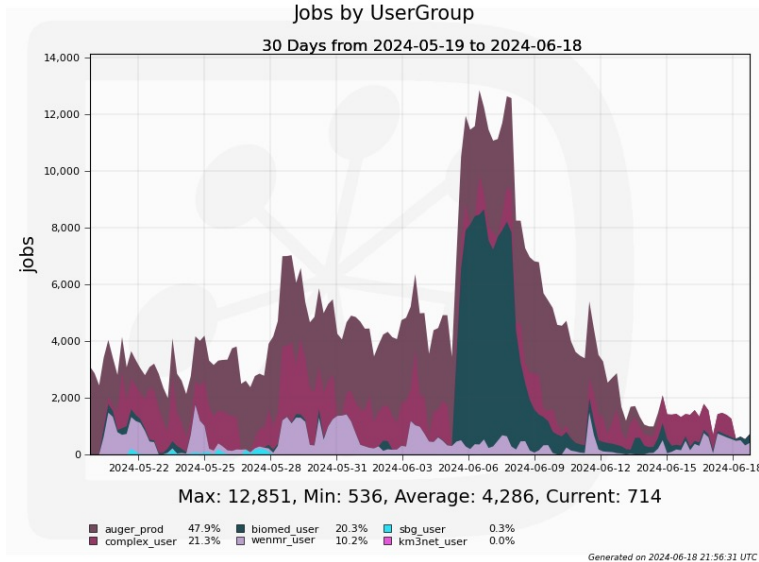
-
- ▶ The EGI DIRAC services are maintained by the members of the DIRAC@IN2P3 Project
 - ▶ CPPM/Marseille, LUPM/Montpellier, CC/IN2P3/Lyon

 - ▶ DIRAC services provided
 - ▶ WMS services
 - ▶ Transformation service is enabled but not much used (demos, training)
 - ▶ DMS services
 - ▶ Multiple FileCatalogs (General, Biomed, Eiscat, HESS, Auger, ...)
 - ▶ RMS
 - ▶ Accounting
 - ▶ Monitoring

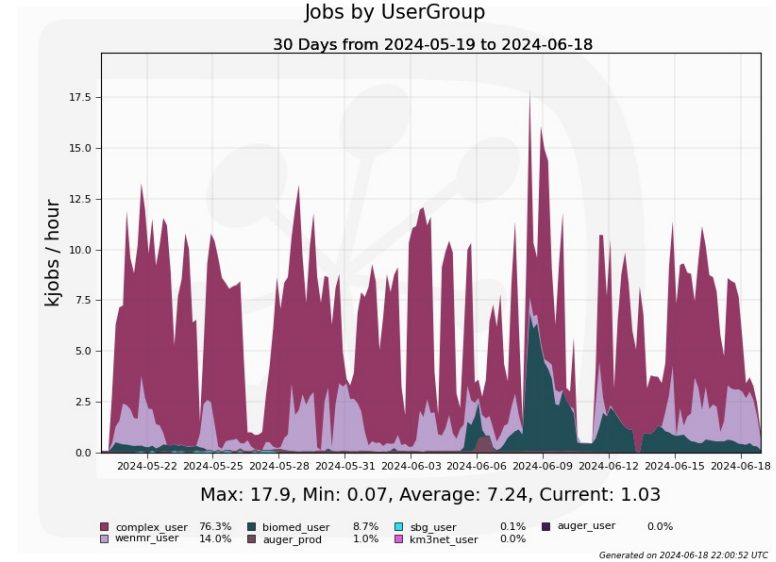
 - ▶ ElasticSearch problems to be still investigated
 - ▶ OpenSearch client incompatibilities ?

Operations: Job execution rates

Running jobs



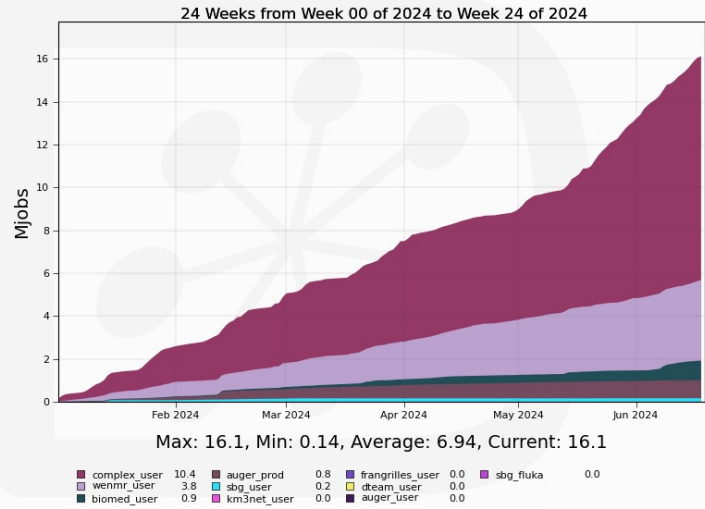
Job Execution rate



- ▶ Up to 5Hz of executed jobs
 - ▶ Up to 200K jobs per day
- ▶ Up to 13K running jobs

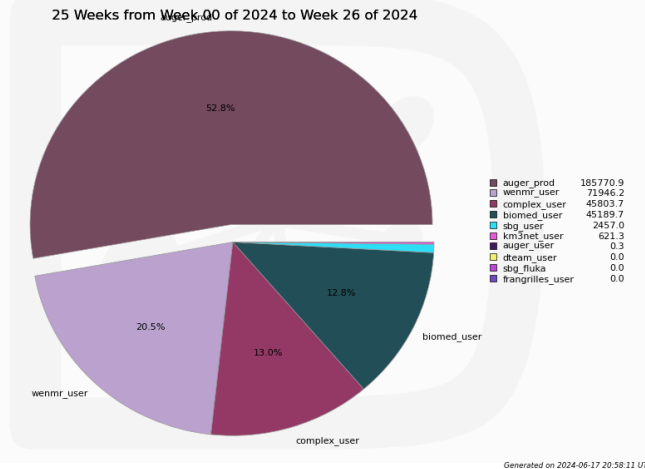
Operations: Workloads executed

Cumulative Jobs by UserGroup

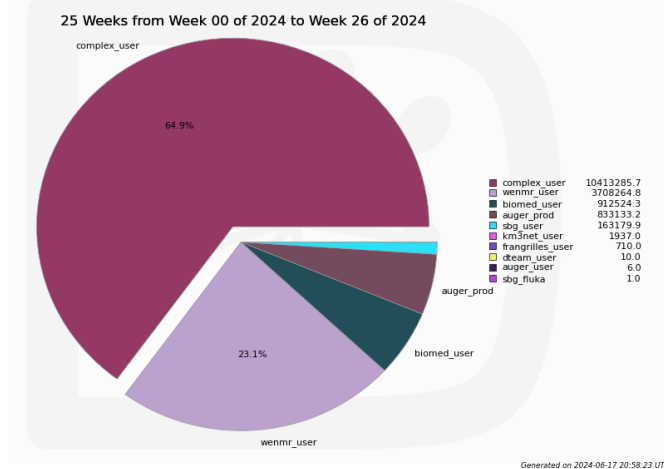


- ▶ 16M jobs since 1 Jan 2024
- ▶ 16m jobs in the whole 2023
- ▶ Very different job patterns
- ▶ Lots of short jobs vs few long jobs

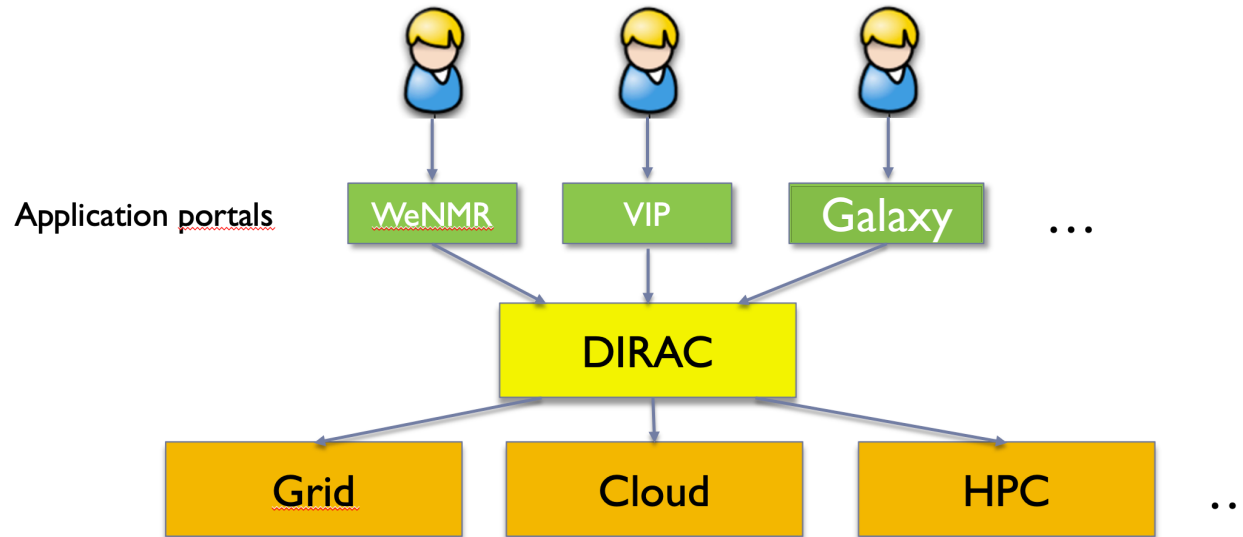
CPU days used by UserGroup



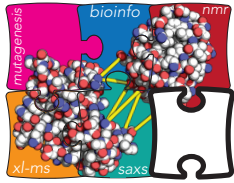
Total Number of Jobs by UserGroup



- ▶ ~20 communities with ~700 registered users
- ▶ Two distinct types of communities
 - ▶ Use of DIRAC by individual users
 - ▶ Auger, HESS, SBG, KM3NeT, biomed, OpenMOLE, ...
 - ▶ Needs more effort for the user support, individual user registration, etc
 - ▶ Application portals between users and the DIRAC service
 - ▶ Users are managed by the portals
 - Registration, profiles, accounting
 - ▶ Portals are represented as a single user to DIRAC
 - Easier case for DIRAC, better synergy



- ▶ WeNMR (<https://wenmr.science.uu.nl/>), Haddock application, protein docking
 - ▶ >44K registered users
- ▶ VIP, medical imaging (<https://vip.creatis.insa-lyon.fr>)
 - ▶ ~1500 users
- ▶ Galaxy, an open source, web-based platform for data intensive biomedical research (<https://usegalaxy.org/>)
 - ▶ Potentially many
 - ▶ Work in progress on the DIRAC job submission (runners)

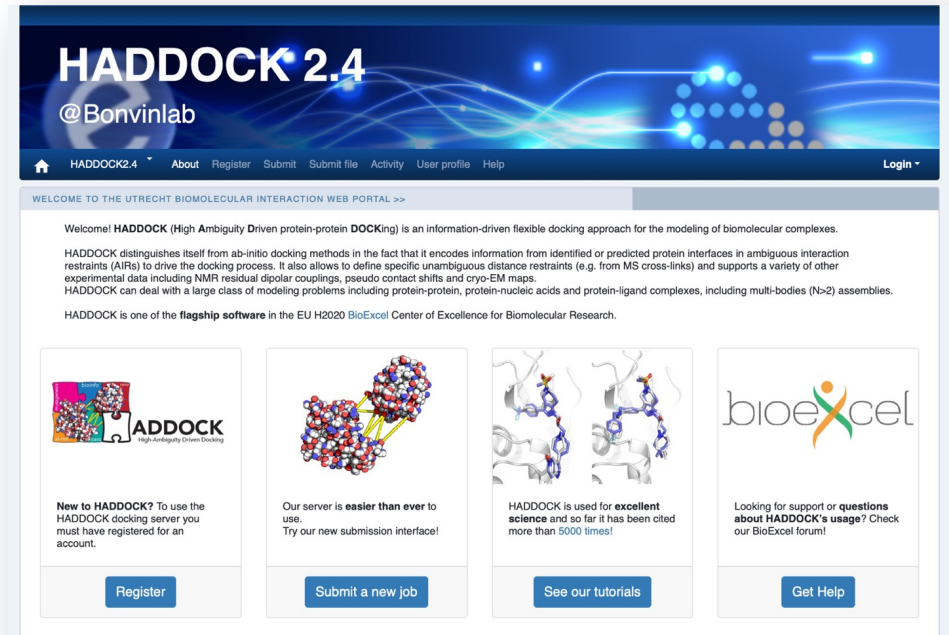


HADDOCK
High-Ambiguity Driven Docking

- > **44600 registered users**
- > **650000 served runs since June 2008**
- **65% on the EOSC HTC resources (>85% for 2.4) using the EGI workload manager (DIRAC)**
- **Integrated in the EOSC marketplace**

De Vries *et al.* Nature Prot. 2010

Van Zundert *et al.* J.Mol.Biol. 2016



HADDOCK 2.4
@Bonvinlab

Home HADDOCK2.4 About Register Submit Submit file Activity User profile Help Login


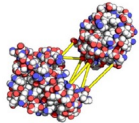
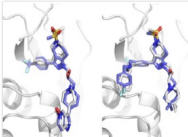

WELCOME TO THE UTRECHT BIOMOLECULAR INTERACTION WEB PORTAL >>>

Welcome! **HADDOCK** (High Ambiguity Driven protein-protein **DOCK**ing) is an information-driven flexible docking approach for the modeling of biomolecular complexes.

HADDOCK distinguishes itself from ab-initio docking methods in the fact that it encodes information from identified or predicted protein interfaces in ambiguous interaction restraints (AIRs) to drive the docking process. It also allows to define specific unambiguous distance restraints (e.g. from MS cross-links) and supports a variety of other experimental data including NMR residual dipolar couplings, pseudo contact shifts and cryo-EM maps.

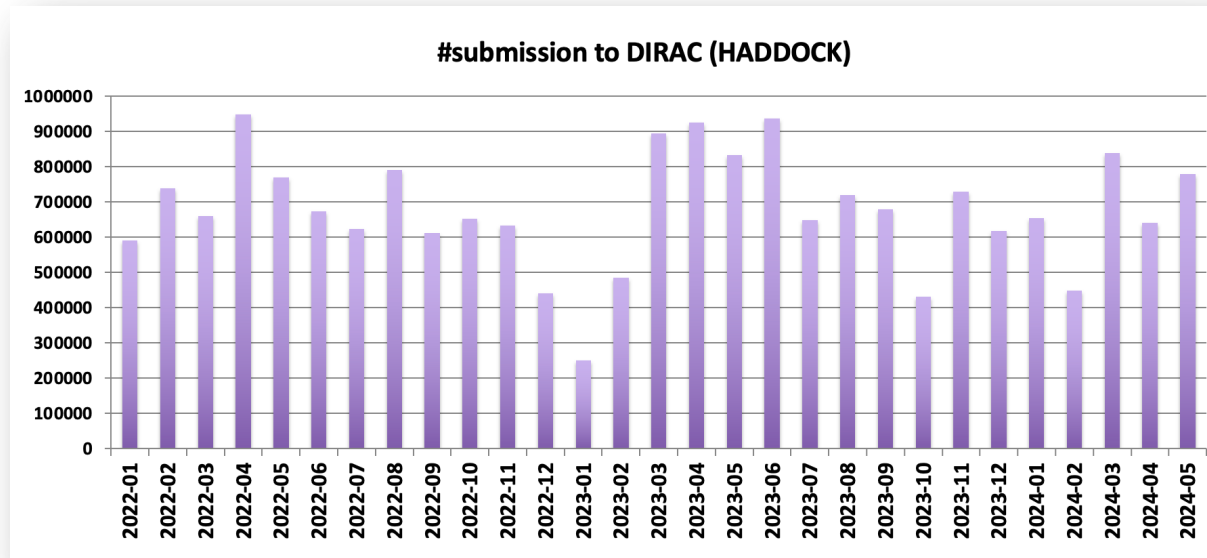
HADDOCK can deal with a large class of modeling problems including protein-protein, protein-nucleic acids and protein-ligand complexes, including multi-bodies (N>2) assemblies.

HADDOCK is one of the **flagship software** in the EU H2020 **BioExcel** Center of Excellence for Biomolecular Research.

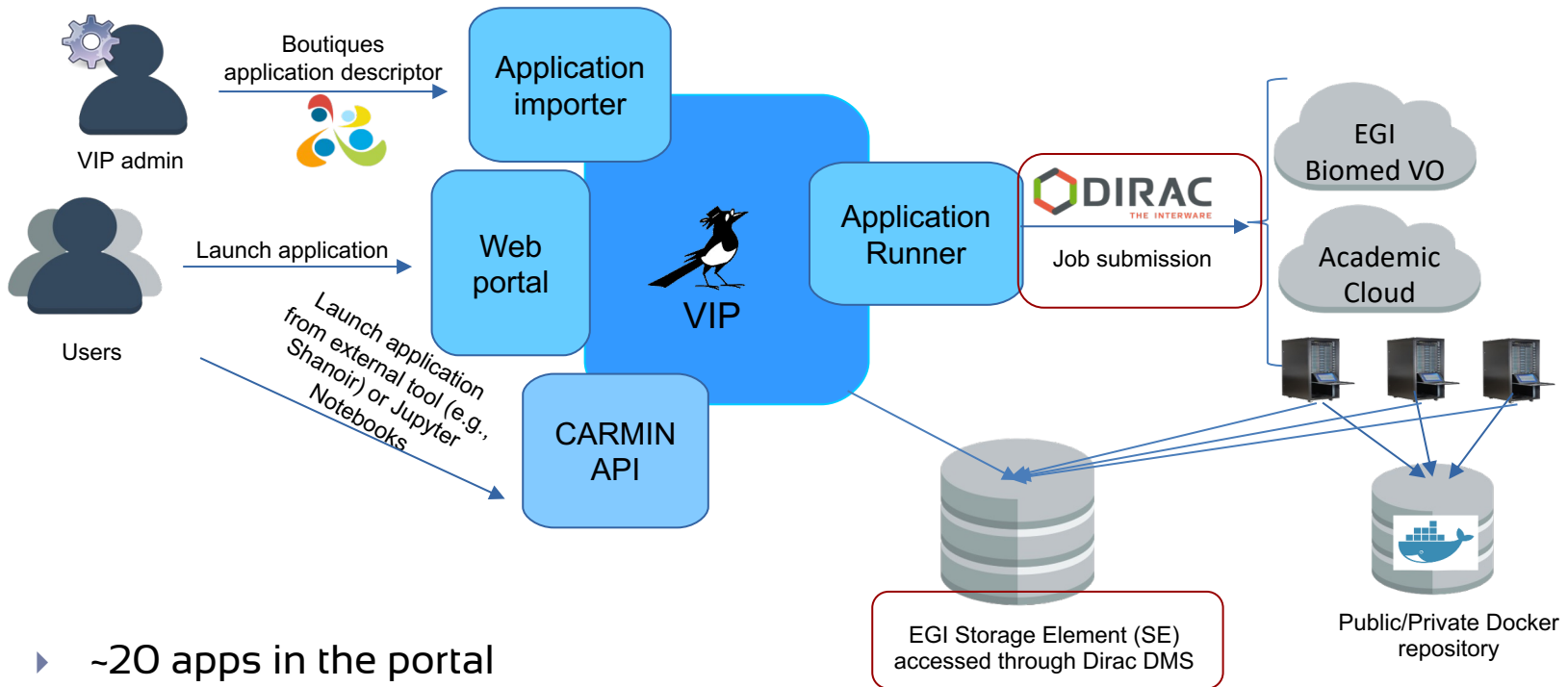
 <p>HADDOCK High-Ambiguity Driven Docking</p> <p>New to HADDOCK? To use the HADDOCK docking server you must have registered for an account.</p> <p>Register</p>	 <p>Our server is easier than ever to use. Try our new submission interface!</p> <p>Submit a new job</p>	 <p>HADDOCK is used for excellent science and so far it has been cited more than 5000 times!</p> <p>See our tutorials</p>	 <p>Looking for support or questions about HADDOCK's usage? Check our BioExcel forum!</p> <p>Get Help</p>
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<https://wenmr.science.uu.nl>

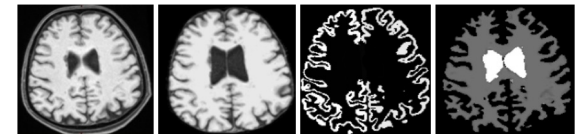
Average of ~675000 job submissions to DIRAC per month by the HADDOCK server



- ▶ Using HTC and Cloud sites
 - ▶ No tokens
- ▶ Smooth running
 - ▶ Few problems with VOMS configuration changes non properly propagated to sites
- ▶ App software from CVMFS
- ▶ Future version of Haddock
 - ▶ will execute complex workflows (MPI) on worker nodes – will require more **cloud** resources
 - ▶ will require different data transfer mechanisms (in/out)



- ▶ ~20 apps in the portal
- ▶ Using HTC and Cloud sites
 - ▶ Using EGI Check-In tokens and VOMS certificates
 - ▶ Dedicated FC and custom services
- ▶ Containerized applications (Docker)
- ▶ Using custom cloud VMs with SSHCE
 - ▶ Accessing GPU's
- ▶ Request for definition of CloudCE queues for VMs with GPU access configured



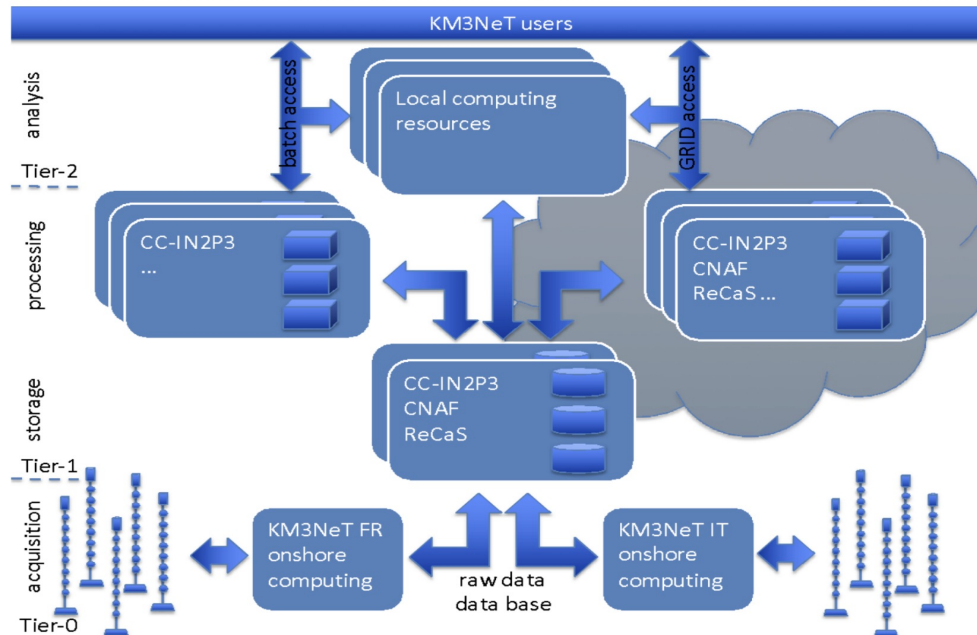
- ▶ Complex systems modeling applications (<https://iscpif.fr/projects/openmole/>)
- ▶ thousands evolutionary algorithms running in parallel (as jobs) orchestrated by a single global algorithm
 - ▶ Resulting in many short jobs in DIRAC
- ▶ Modeling software in different languages (java, scala, ...)
 - ▶ Using REST (ancient !) DIRAC interface
- ▶ Requests:
 - ▶ REST interface for both jobs and data
 - ▶ Most impassionate potential DiracX users !
 - ▶ Both data bookkeeping and data access (webdav)
 - ▶ Moving to use tokens – to be quickly done for jobs. For data – to be seen
 - ▶ User management with Check-In is to be set up



- ▶ Pierre Auger Observatory
 - ▶ Running heavy MC data productions with the EGI DIRAC services on HTC resources
 - ▶ Peculiarities:
 - ▶ Dedicated FC managed and hosted on the community server *dfc-auger.grid.cesnet.cz*
 - ▶ Using **Perun** user management service
 - ▶ See *Jiri's presentation*



- ▶ The KM3NeT is a large Research Infrastructure (RI) that will consist of a network of deep-sea neutrino detectors in the Mediterranean Sea
- ▶ Tier structure of the Computing Model



- ▶ Starting with the EGI DIRAC service
 - ▶ MC production
 - ▶ Mass Data Processing
- ▶ Currently all workflows are implemented in the Snakemake workflow engine <https://snakemake.github.io/>
 - ▶ Job submission to DIRAC
- ▶ User and community management in an Indigo IAM service
 - ▶ Should benefit from multi-IdP support in DIRAC
- ▶ Setting up Rucio service for data management
 - ▶ DIRAC-Rucio bundle is becoming more and more popular
- ▶ Looking at organizing mass productions with the DIRAC TS
- ▶ Problems encountered:
 - ▶ The DiracOS2 not well implemented on arm architecture when running on local osx client.
 - ▶ Need Admin access to see Accounting for jobs of all the VO users – need VOAdmin level privileges.
- ▶ Wish list:
 - ▶ KM3NeT Dirac/Rucio container standalone
 - ▶ Integration between Dirac Transformation System and Rucio
 - ▶ Better documentation ☺

- ▶ The CVMFS dirac.egi.eu repository is maintained
 - ▶ Admins: Andrei, Daniela
- ▶ The repository is updated automatically nightly:
 - ▶ DIRACOS2 installers
 - ▶ Pilot files
- ▶ The DIRAC clients for 8.* and 9.* releases are installed automatically (github action)
 - ▶ Backed up by a cronjob
 - ▶ Intel and ARM versions
- ▶ Unstable behavior
 - ▶ Problems with Ceph mounted FS:
 - ▶ Failures in releases installations
 - ▶ Slow publishing to CVMFS clients
 - ▶ Managers are trying to cope but with a limited success so far

- ▶ Stable EGI DIRAC service operation with increasing numbers of payloads

- ▶ New communities are showing interest in the service and need guidance

- ▶ Points of user's interest
 - ▶ Token based user management (Check-In, IAM)
 - ▶ More versatile use of Cloud resources
 - ▶ Looking for DIRAC-Rucio combined services