Cloud & HTC infrastructure integration workshop

BITP

Sergiy Svistunov, Volodymyr Yurchenko

Bogolyubov Institute for Theoretical Physics of the NAS of Ukraine

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Recipient Party: Project consortium

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BITP Cloud infrastructure

In 2015 the first OpenStack site at Bogolyubov Institute for Theoretical Physics (BITP) of the National Academy of Sciences (NAS) of Ukraine was put into operation.

For the first installation, we used old servers with configuration: Intel Xeon CPU E5335 2.00GHz (8 core), RAM 8 Gb, HDD 450 Gb. In this configuration, it was impossible to make full use of the cloud cluster in scientific computing.

However, it is allowed to start user training, to start experiments on the implementation of cloud computing in scientific projects, and then to register BITP cloud site in EGI Federated Cloud.

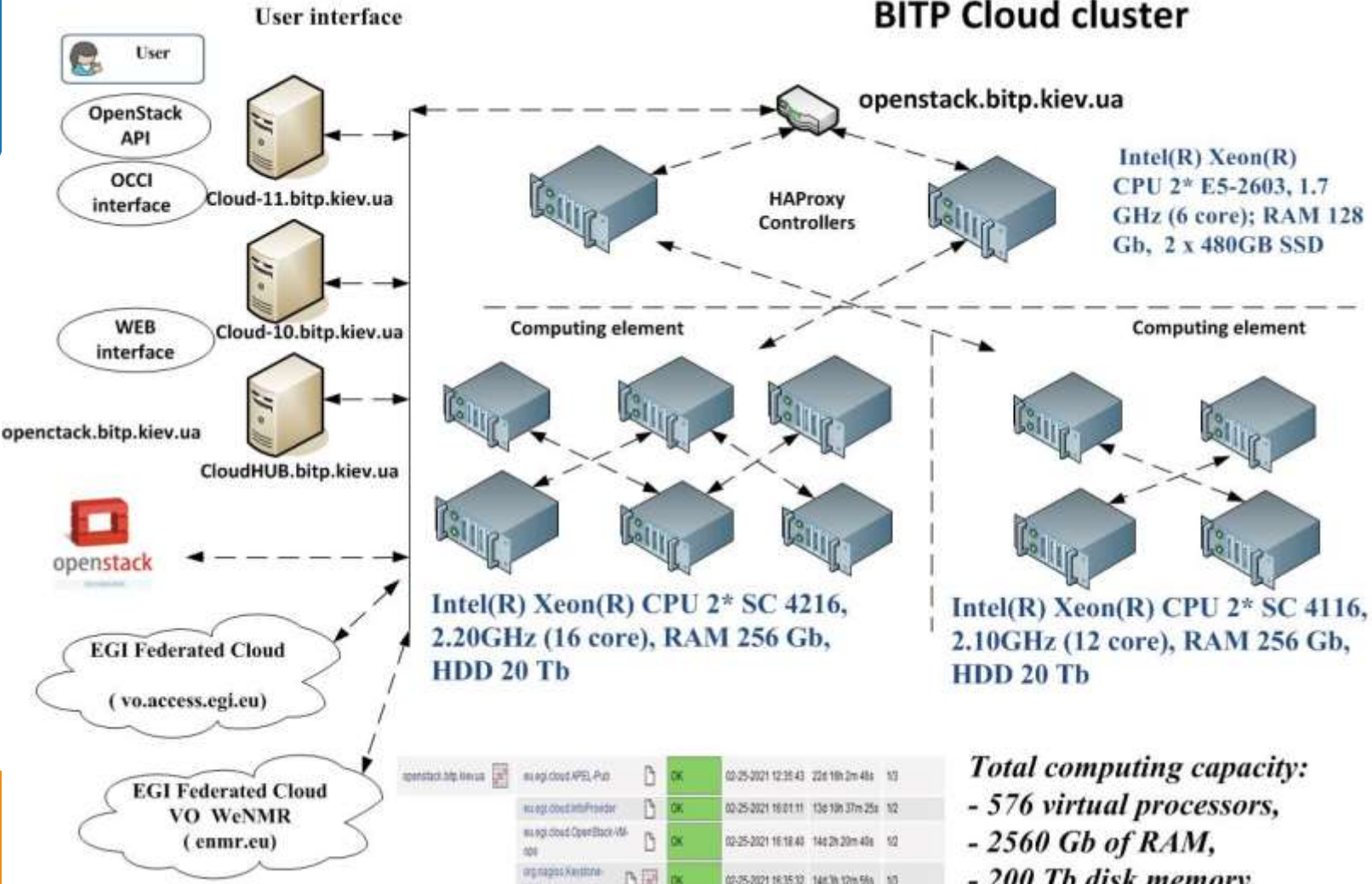
Current BITP Cloud infrastructure

In 2019 the BITP cloud cluster was migrated to modern servers, which significantly expanded its computing capacity and facilitated its usage in the scientific projects.

The main purpose of the cloud project in BITP: usage of cloud technologies for scientific computing at the National Academy of Sciences of Ukraine, user training, building a cloud computing resource center under the requirements of EGI Federated Cloud.

Until 2020, the BITP cloud cluster was the only one resource center in Ukraine that was registered in the EGI Federated Cloud.

BITP Cloud cluster



Total computing capacity:
- 576 virtual processors,
- 2560 Gb of RAM,
- 200 Tb disk memory.

Cloud computing in Ukraine

The main problem is that cloud technologies have not yet become a toolkit for scientific computing in Ukraine.

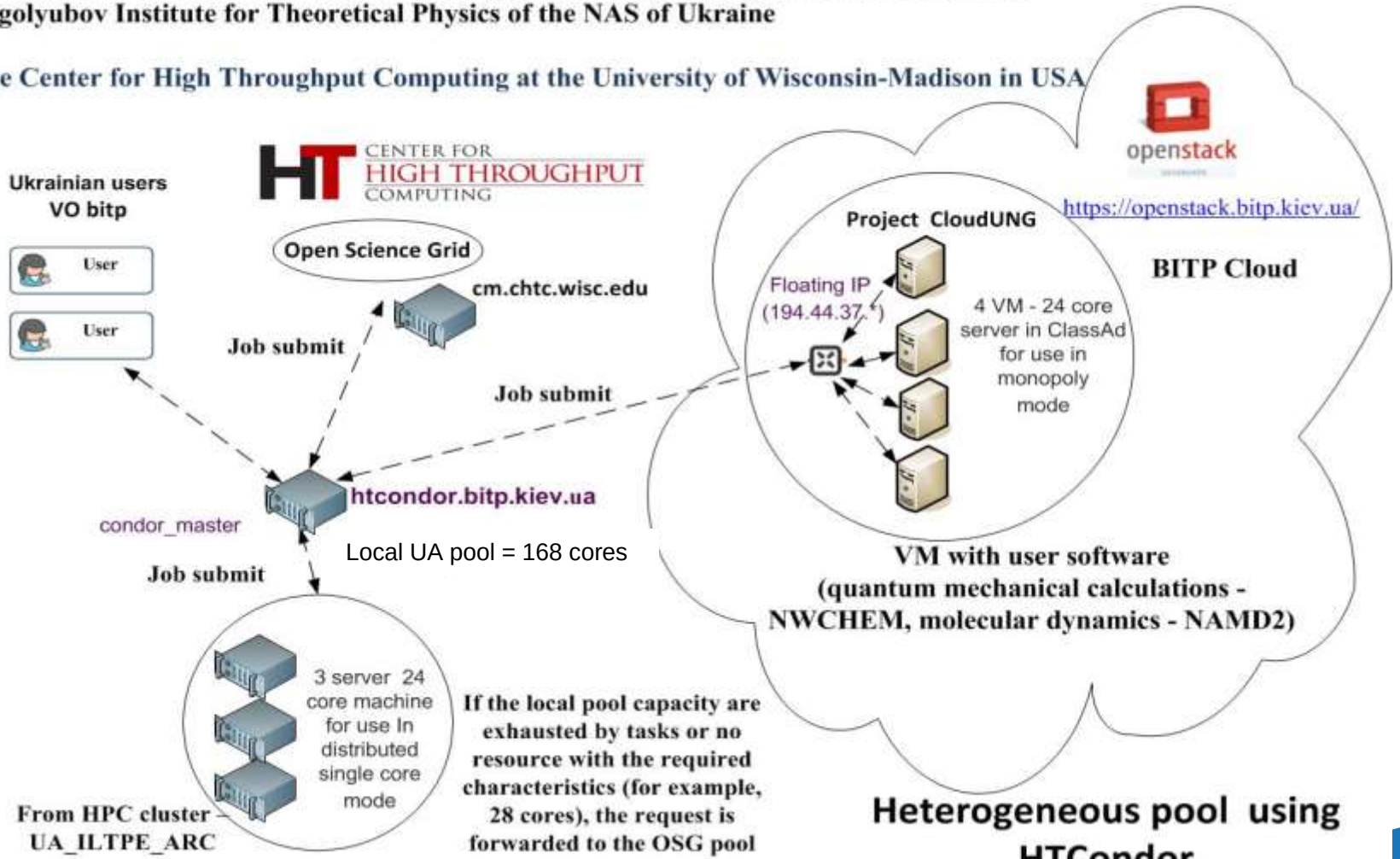
The reason for this situation is that users mainly use cluster technologies and, to a lesser extent, grid technologies.

The use of cloud technologies requires some preliminary action: writing contextualization files, learning the methods of the software installation on the virtual servers and some corrections to the application program code. This requires an effort from the users that they don't want to make.

The projects that are currently implemented in the BITP cloud are focused on local scientific research activities at the National Academy of Sciences of Ukraine.

B.Verkin Institute for Low Temperature Physics and Engineering of the NAS of Ukraine
Bogolyubov Institute for Theoretical Physics of the NAS of Ukraine

The Center for High Throughput Computing at the University of Wisconsin-Madison in USA



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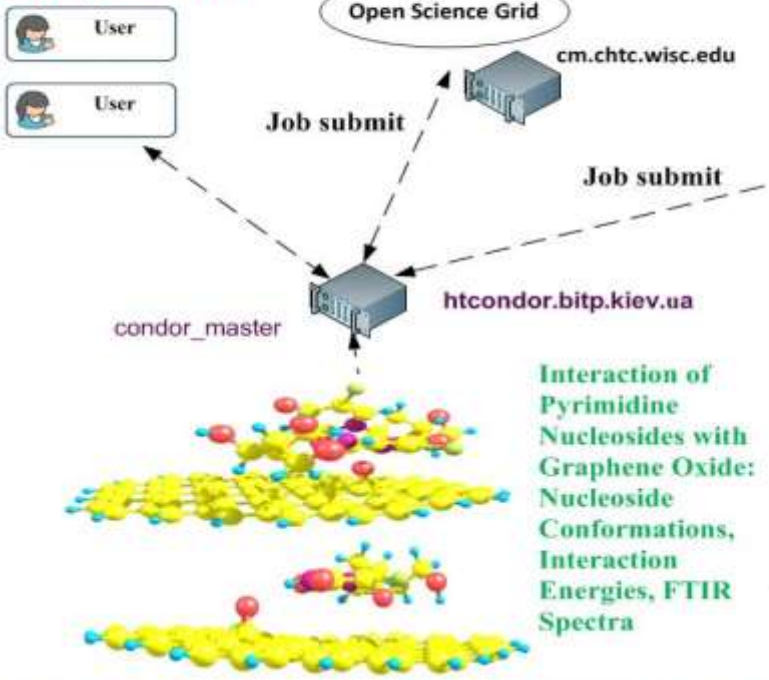
The Center for High Throughput Computing at the University of Wisconsin-Madison in USA

openstack

https://openstack.bitp.kiev.ua/

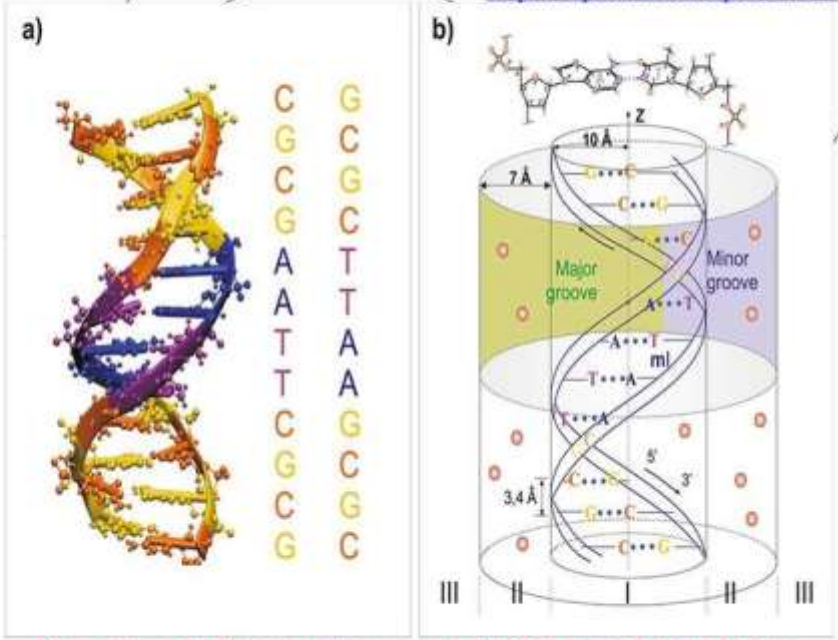
Two groups of researchers
VO bitp - 4 users

CENTER FOR HIGH THROUGHPUT COMPUTING



Interaction of Pyrimidine Nucleosides with Graphene Oxide: Nucleoside Conformations, Interaction Energies, FTIR Spectra

Molecular structure and energy of vertical interaction (Eint) in the complex of deoxy 5-bromuridine with a fragment of oxygraphene

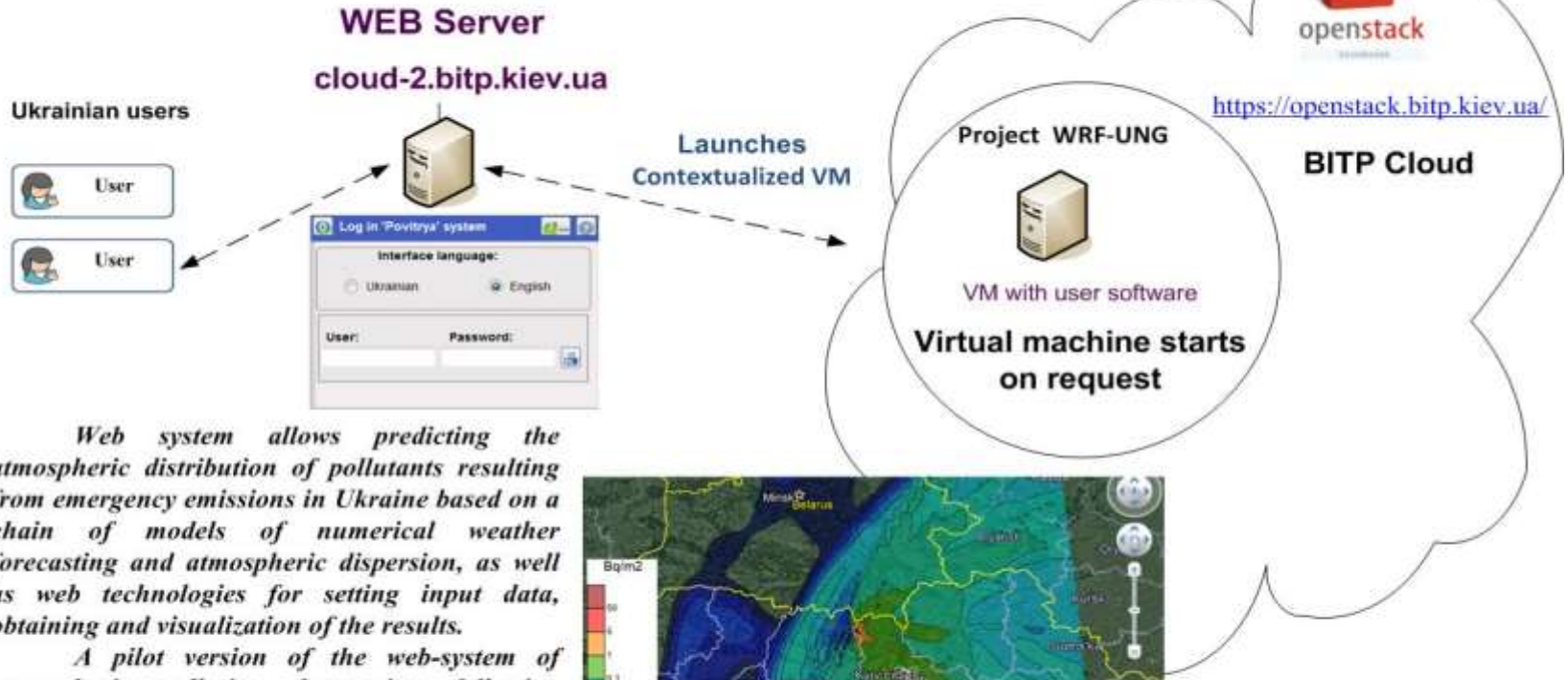


Dynamics of K^+ counterions around DNA double helix in the external electric field: A molecular dynamics study

https://link.springer.com/article/10.1140%2Fepje%2Fi2020-12000-077

In 2020 year - Local pool: 125,428 core-hours
CHTC pool: 43,653 core-hours

Institute of Mathematical Machines and Systems Problems NAS of the Ukraine
Bogolyubov Institute for Theoretical Physics of the NAS of Ukraine



Web system allows predicting the atmospheric distribution of pollutants resulting from emergency emissions in Ukraine based on a chain of models of numerical weather forecasting and atmospheric dispersion, as well as web technologies for setting input data, obtaining and visualization of the results.

A pilot version of the web-system of atmospheric pollution forecasting following accidental release in Ukraine was created and installed for test operation . The atmospheric dispersion model CALPUFF is configured to calculate the transport of three main types of pollution: aerosols, gases and passive tracer.

Calculated the total loss distribution of Cs-137 during the fires in the Chernobyl exclusion zone in April 2020

National Technical University of Ukraine “Igor Sikorsky Kyiv Polytechnic Institute”
Bogolyubov Institute for Theoretical Physics of the NAS of Ukraine

In 2020, 135 students were trained

cloud-11.bitp.kiev.ua

Launches Contextualized VM

User

openstack

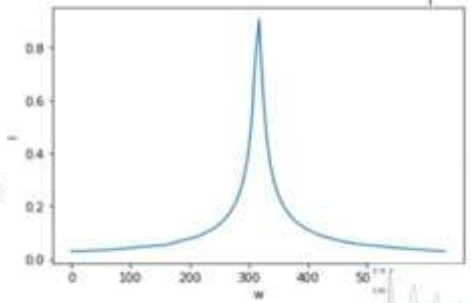
https://openstack.bitp.kiev.ua/

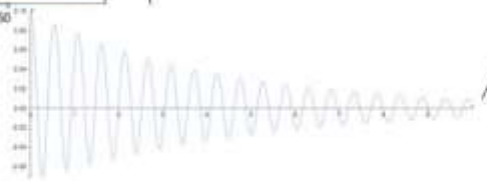
Project CloudKPI

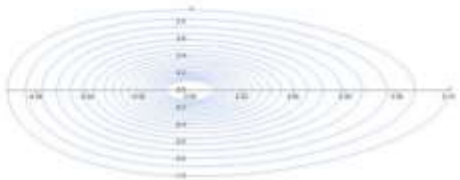
BITP Cloud

VM with user software

Virtual machine starts on request







Education assistance project

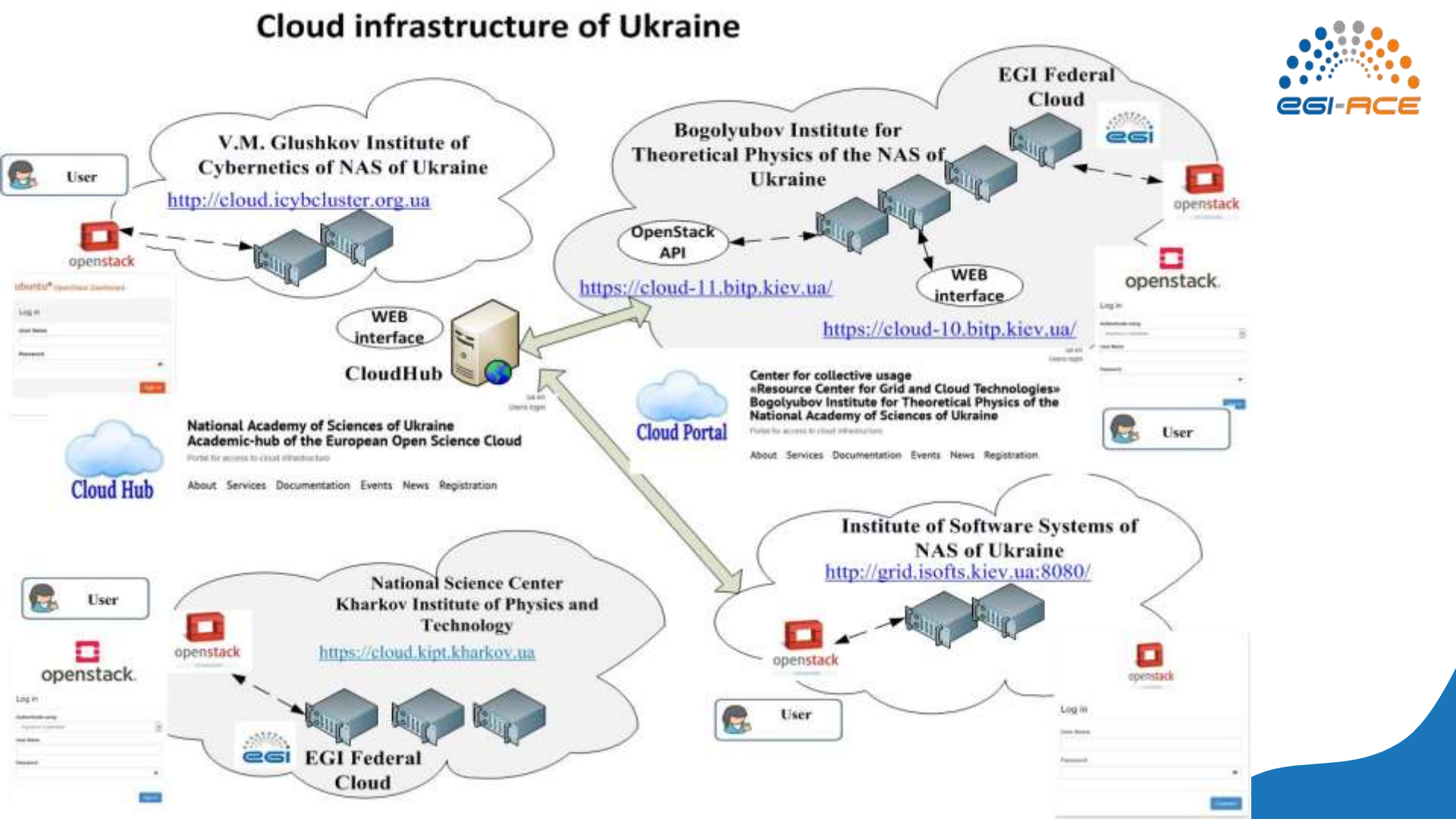
Goal: To support students in their laboratory assignments at the studying courses "*Cloud and Grid technology*" and "*Grid technologies for distributed computing and data processing*"

Current activities

- Lectures and seminars to promote cloud technologies among users in the NAS of Ukraine.
- A website were implemented the basic functions for working with a virtual server and it was like a simplified version of the Openstack dashboard. However, the users of this site are mainly researchers of our institute.
- Installations of OpenStack clouds in three other institutes of the NAS in 2019 - 2020's (as part of a local grand).
- In 2020, the CloudHUB project was started.

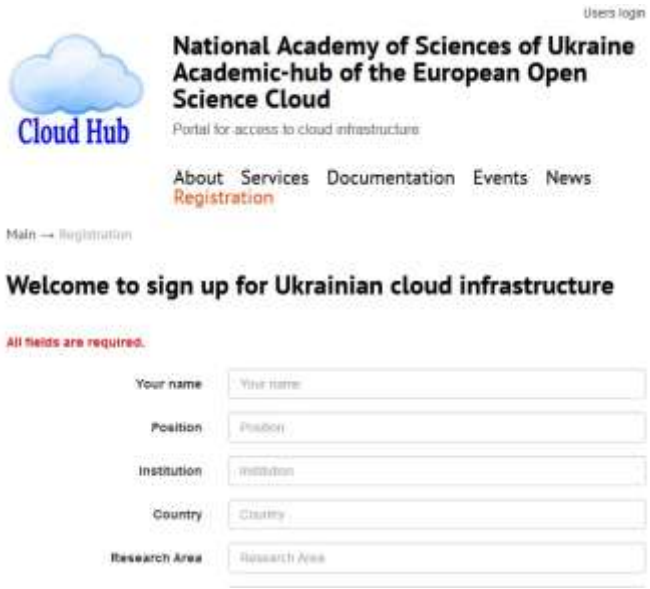
The purpose of CloudHUB project is to minimize the efforts for access to existing cloud infrastructure for users from the institutes of the National Academy of Science, to make a single point of access to cloud clusters and to provide a common pool of cloud resources to support the local research projects.

Cloud infrastructure of Ukraine



BITP Cloud infrastructure

Users from the institutes of the National Academy of Sciences can create a new project and get access to the cloud resources to run their software.



CloudHUB implements all basic functions for managing virtual servers and virtual disks. In 2020, two cloud clusters (BITP, IPS) were connected to the CloudHub. Currently, CloudHUB works in a test mode.

Evolution of CloudHUB project

Next steps:

- increase computing capacity of the local common cloud pull;
- connect more cloud clusters;
- support EGI Check-in;
- add new features in CloudHUB, in particular, a library of images of virtual servers;
- actively promote the CloudHUB among the users in the Academy.

Support of EGI services

BITP cloud operators already have some experience in running some of the integration services :

- **EGI Check-in** is set up as an alternative to name-password login
  - added as a plug-in to OpenStack Keystone (authorization service) and Horizon (dashboard service);
- **AppDB** image lists configured for *vo.access.egi.eu* and *WeNMR* VOs
  - synchronized via cloudkeeper service;
- **CVMFS** client installed in a Virtual Machine by the contextualization scripts
  - tested on the computational VMs for ALICE experiment at CERN;
  - we had a local CVMFS cache server (powered by Squid);
- **CASO** – accounting tool for OpenStack
  - runs in a Docker container.

Thank you!

Contact: **egi-ace-po@mailman.egi.eu**
Website: **www.egi.eu/projects/egi-ace**

EGI Foundation

@EGI_eInfra

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