

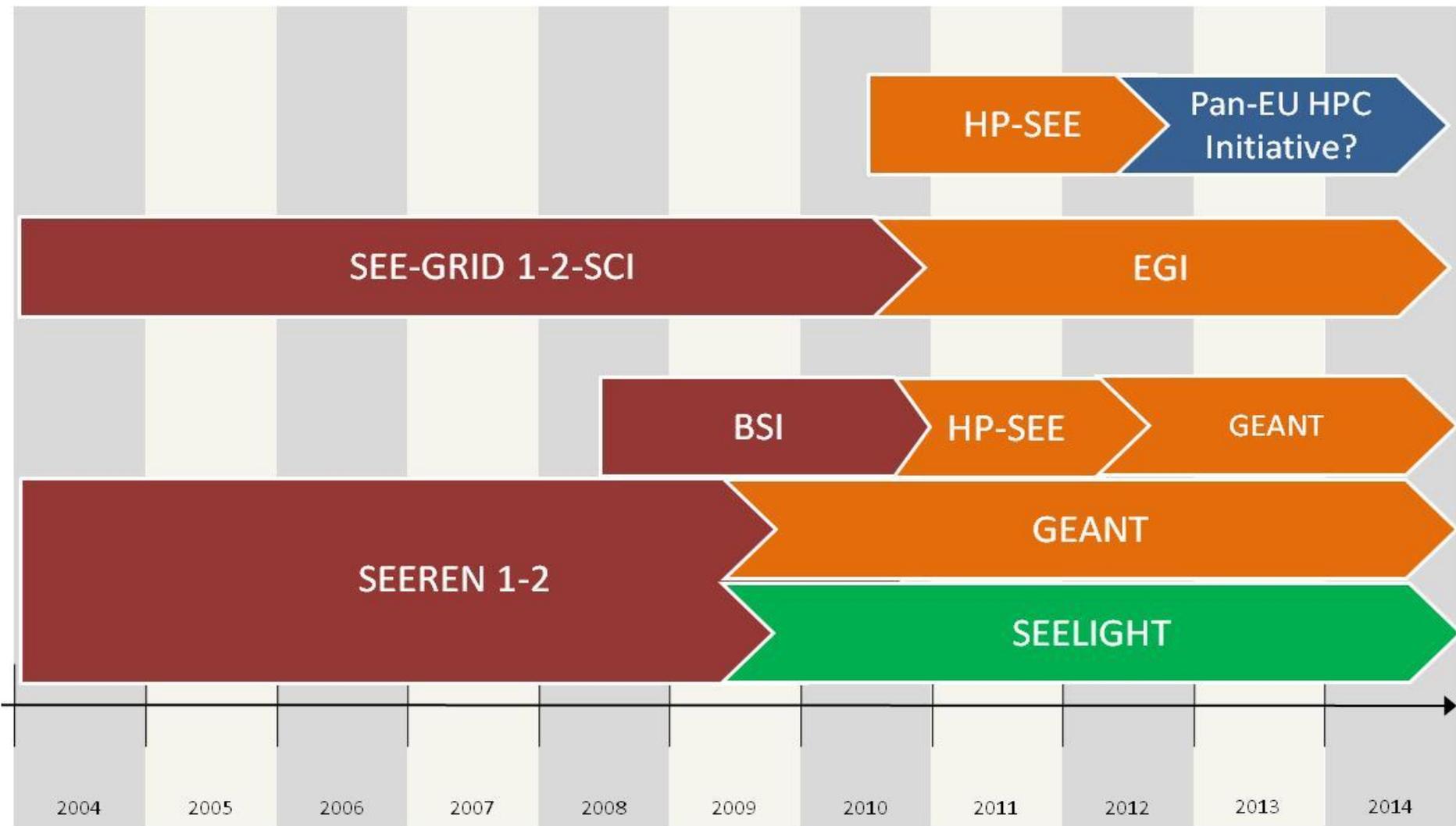
**VI-SEEM services for the Scientific
Communities: Life Sciences,
Climatology and Digital Cultural
Heritage**

**VI-SEEM National Dissemination Event
Sofia, 3 Nov 2016**

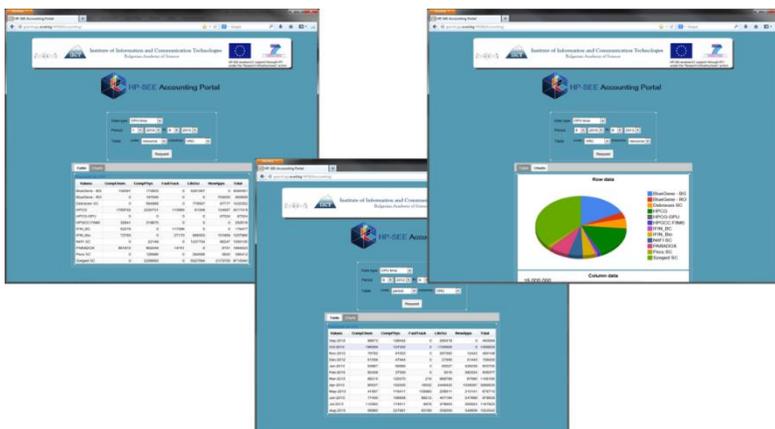
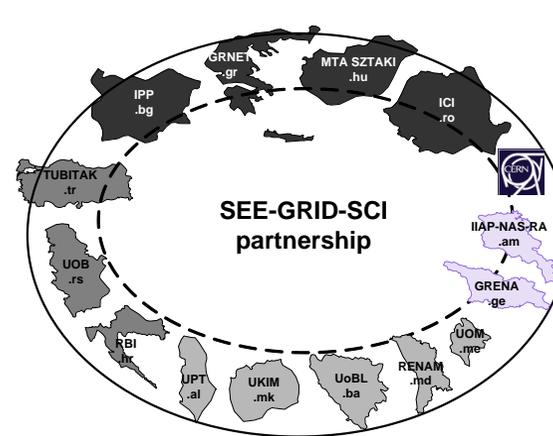
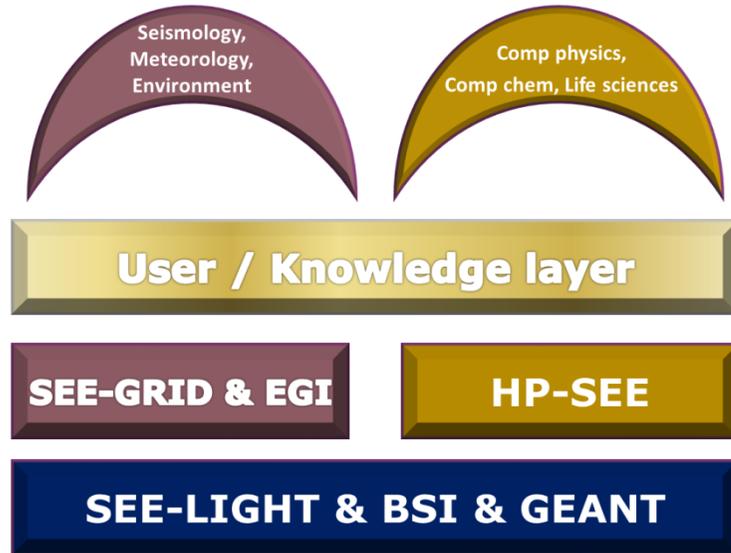
E. Atanassov
IICT-BAS



Regional cooperation history



Regional partnerships – from infrastructure to applications



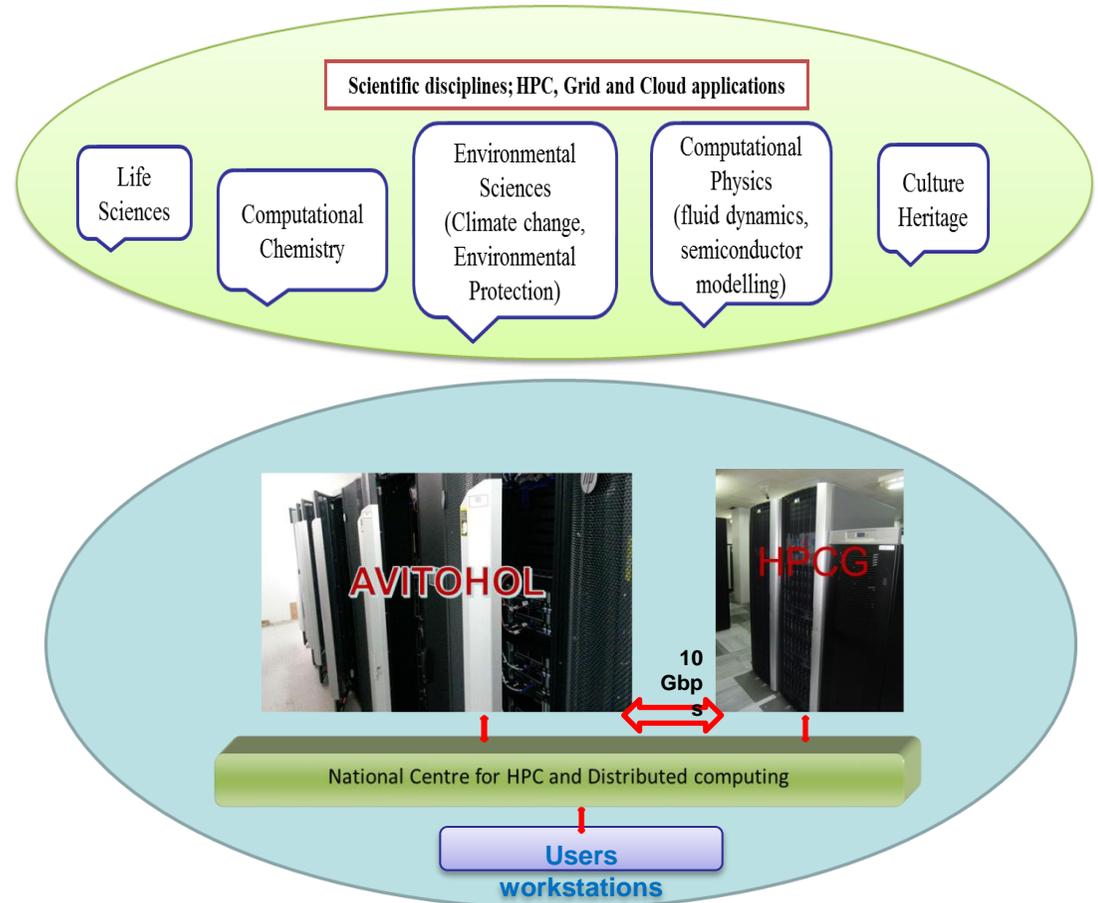
HPC Center “Avitohol” at IICT

150 HP Cluster Platform SL250S GEN8 servers
with 2 Intel Xeon E 2650 v2 CPUs and 2 Intel Xeon
Phi 7120P coprocessors

Site	IICT-BAS/Avitohol
Manufacturer	Hewlett-Packard
Cores	20700
Interconnection	FDR InfiniBand
Theoretical Peak Performance	412.3 Tflop/s
RMAX Performance	264.0 Tflop/s
Memory	9600 GB
Operation System	Red Hat Enterprise Linux for HPC
Storage capacity	96 TB SAN

Top500 List on 389 place (Nov 2015)

<http://www.top500.org/system/178609>



The Supercomputer System Avitohol at IICT-BAS

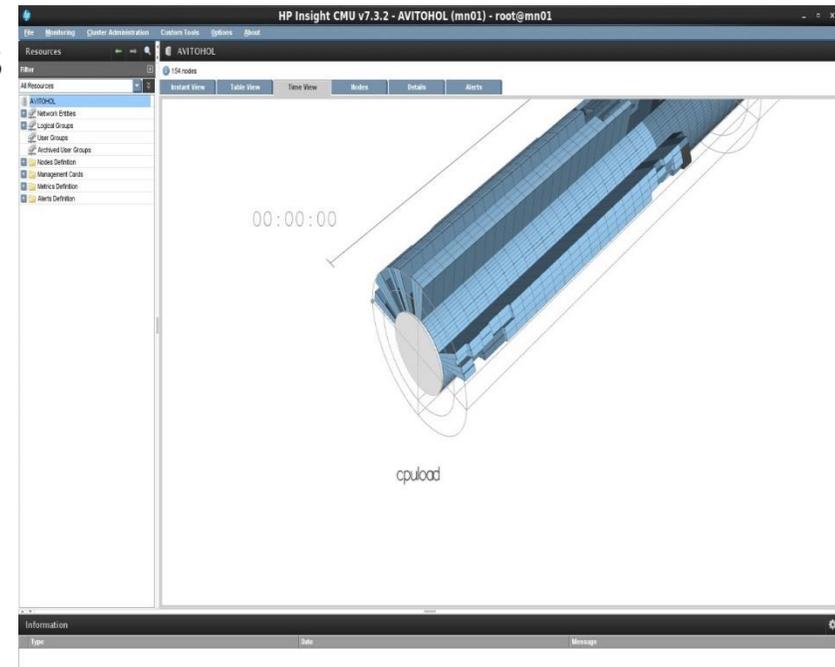


- ❑ 8 water-cooled racks of type HP MCS 200, paired in couples.
- ❑ Each pair provides power and cooling for up to 50 kW of equipment
- ❑ About 90% of the computational power comes from the accelerators – one 7120P coprocessor achieves 1.25 TFlop/s in double precision.
- ❑ Total energy use at maximum load ~ 250kW.



The Supercomputer System Avitohol at IICT-BAS

- ❑ RedHat Enterprise for HPC
- ❑ Intel Cluster Studio (compilers, MPI, MKL)
- ❑ Moab for resource management with web and command line interface
- ❑ High-end database software - SAP HANA – in-memory database with advanced real-time analytics capabilities
- ❑ 150 dual-socket nodes HP SL250s Gen8 with 2 Intel Xeon E5-CPU E5-2650 v2 @ 2.60GHz and 2 Intel Xeon Phi 7120P coprocessors, 64 GB RAM
- ❑ Interconnected with fully non-blocking FDR InfiniBand
- ❑ Lustre parallel filesystem, 96 TB of disk storage



HPC resources in Bulgaria

AVITOHOL at IICT-BAS

150x HP ProLiant SL250s Gen8 each with
2x Intel Xeon E5-2650 v2 (8C/16T),
64 GB DDR3-1866 RAM and
2x Intel Xeon Phi 7120P
6x HP ProLiant DL380p Gen8 nodes with
2x Intel Xeon E5-2650v2 (8C/16T),
64 GB DDR3-1866 RAM
Infiniband 56 Gb/s FDR
Storage system with 96 TB



Total Performance:
RPeak: 412.3 TFlop/s
RMax: 264.2 TFlop/s
Top 500 position: 389

HPCG cluster at IICT-BAS

36 blades BL 280c(2x Intel X5560(4C/8T); 24GB DDR3);
8 management nodes HP DL 380 G6(2x Intel
X5560(4C/8T); 32GB DDR3);
2 HP ProLiant SL390s G7(2x Intel E5649(6C/12T);96GB
DDR3)
8x nVidia TESLA M2090 per server;
2 HP SL270s Gen8 (2x Intel Xeon E5-2650 v2(8C/16T);
128GB DDR3)
Total number of Xeon Phi 5110P coprocessors: 9
Total 132TBs of system storage



TOTAL PERFORMANCE:
RPEAK: 22.94 TFlop/s

PHYSON at Sofia University

53 Intel Xeon x86_64 processors
524Gibs of system memory
6.5TBs of system storage
2x nVidia Tesla M2090 graphics processors



TOTAL PERFORMANCE:
RPEAK: 3.57 TFlop/s
RMAX: 3.22 TFlop/s

NCSA IBM Blue Gene/P

8192 PowerPC 450 processors
4TBs of system memory
12TBs of system storage
IBM proprietary interconnect with
2.5 μ s latency and 10GBps bandwidth

TOTAL PERFORMANCE:
RPEAK: 27.85 TFlop/s
RMAX: 23.45 TFlop/s



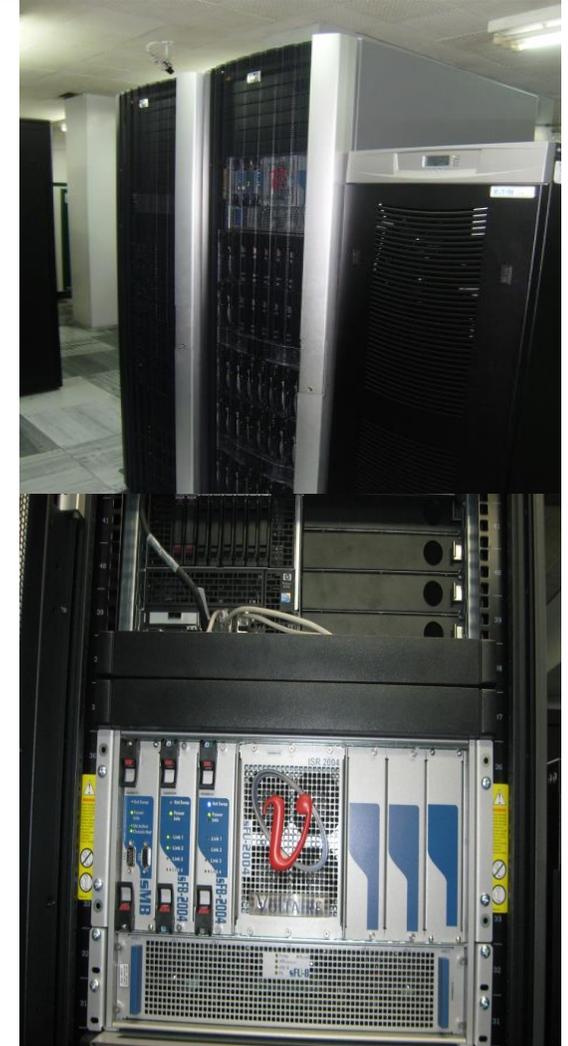
MADARA at IOCCP-BAS

54 Primergy RX200 S5 servers with
2 Intel Xeon E5520(4C/8T) each
and a total of 800GB DDR3 1066MHz
20Gb/s DDR Infiniband
108TB System Storage by Fujitsu FibreCat SX100



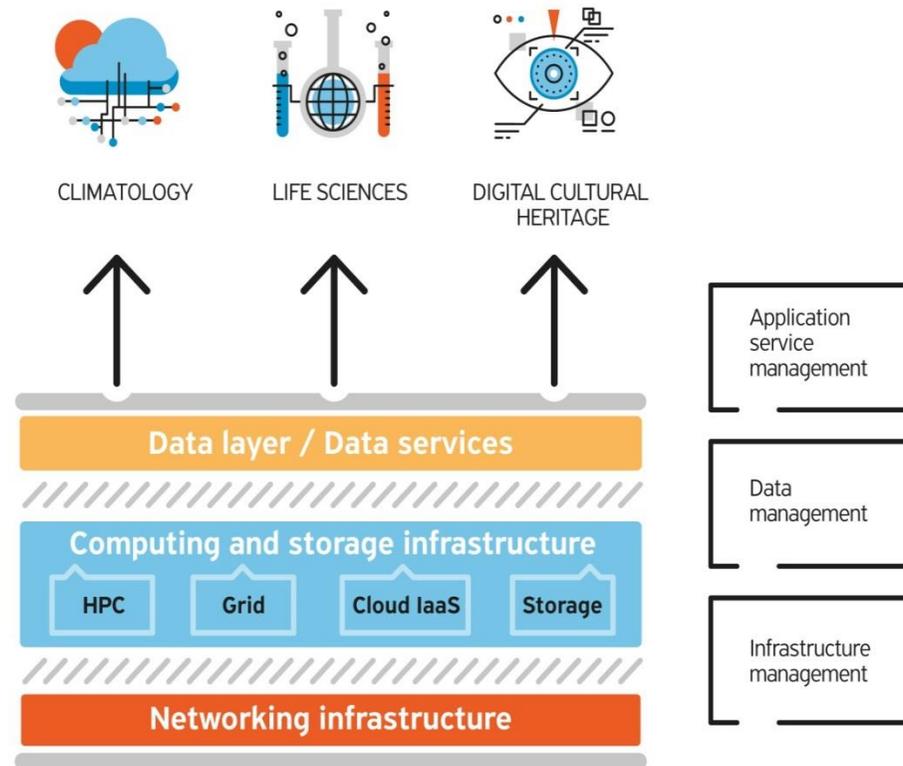
Extension HPCG cluster at IICT-BAS

- ❑ 36 blade servers HP BL 280c, deployed in 3 HP Cluster Platform Express 7000 enclosures, each with 2 Xeon X5560 @ 2.80GHz, 24 GB RAM – 576 cores total with more than 3 Tflops peak performance; 8 dual-socket HP DL 380 G6 with dual Intel X5560 @ 2.8 Ghz, 32 GB RAM. Non-blocking Infiniband interconnection @ 20 Gbps, 92% efficiency on LINPACK
- ❑ Total disk storage more than **132 TB** from three disk systems, interconnected with Fibre Channel.
- ❑ 2 HP ProLiant SL390s G7 4U servers with 16 NVIDIA Tesla M2090 graphic cards (total **8192 GPU cores** with **10.64 TFlops** in double precision); HP SL270s Gen8 4U server with 8 Intel Xeon Phi 5110P Coprocessors (total **480 cores**, 1920 threads, **8.088 TFlops** of double-precision peak performance per server).
- ❑ Total peak theoretical peak performance **22.93 TFlops**



VI-SEEM technology context

- **Overall objective:** Provide user-friendly integrated e-Infrastructure platform for Scientific Communities in **Climatology, Life Sciences and Digital Cultural Heritage** for the SEEM region; by linking compute, data, and visualization resources, as well as services, software and tools
- **Diverse computing technologies**
- **Advent of big data**
- **Service orientation**



VI-SEEM HPC Resources



- HPC Resources (KPI: 21,500 CPUs; 325,000 GPUs; 18,500 Phis)

Resource	Country	Total			Dedicated		
		CPU-cores	GPU-cores	Phi-cores	CPU-hours	GPU-hours	Phi-hours
ARIS	Greece	8,520	-	-	3,000,000	-	-
Cy-Tera	Cyprus	1,392	16,128	-	1,829,088	21,192,192	-
Avitohol	Bulgaria	2,400	-	18,300	2,102,400	-	16,030,800
PARADOX	Serbia	1,696	108,544	-	742,848	47,542,272	-
NIIFI SC	Hungary	768	-	-	421,882	-	-
Leo	Hungary	1,344	628,992	-	588,672	275,498,496	-
InfraGRID	Romania	456	3,136	-	350,400	5,494,272	-
ICAM	Romania	4,096	-	-	7,176,192	-	-
UPT-HPC	Albania	144	-	-	126,144	-	-
FINKI	FYROM	768	-	-	336,384	-	-
Armcluster	Armenia	128	-	-	112,128	-	-
BA-HPC	Egypt	1,040	-	-	1,822,080	-	-
Gamma	Jordan	8	2,496	-	70,080	21,864,960	-
Zaina	Jordan	56	-	-	147,168	-	-
Total		22,816	759,296	18,300	19,273,978	367,353,754	16,030,800

VI-SEEM Cloud Resources



□ Cloud resources (KPI: 10,500 VMs)

Resource	Country	Total VMs	Dedicated VMs	Dedicated VM-hours
~Okeanos	Greece	10,000	200	1,752,000
CyI Cloud	Cyprus	176	18	157,680
Avitohol	Bulgaria	2,400	120	1,051,200
InfraGRID Cloud	Romania	400	46	402,960
UPT-Cloud	Albania	12	6	52,560
ETFBL-CC01	BIH	60	13	113,880
MK-04-FINKI_CLOUD	FYROM	436	24	210,240
MD-Cloud	Moldova	12	3	26,280
IIAP Cloud	Armenia	96	10	87,600
IUCC InfinityCloud	Israel	560	28	245,280
Total		14,152	468	4,099,680

VI-SEEM Grid Resources



□ Grid resources (KPI: 2,900 CPUs)

Resource	Country	Total CPU-cores	Dedicated CPU-cores	Dedicated CPU-hours
Hellas Grid	Greece	864	43	370,000
BG01-IPP	Bulgaria	2,400	120	1,051,200
AEGIS01-IPB-SCL	Serbia	704	35	308,352
MK-03-FINKI	FYROM	768	38	336,384
MREN01CIS	Montenegro	32	16	140,160
MD-GRAP	Moldova	40	12	105,120
GE-01-GRENA	Georgia	64	20	175,200
Total		4,872	284	2,486,416

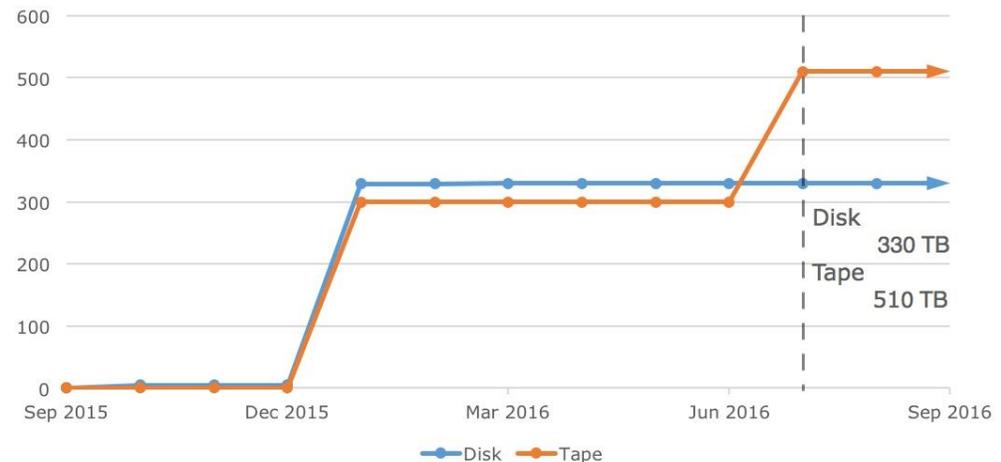
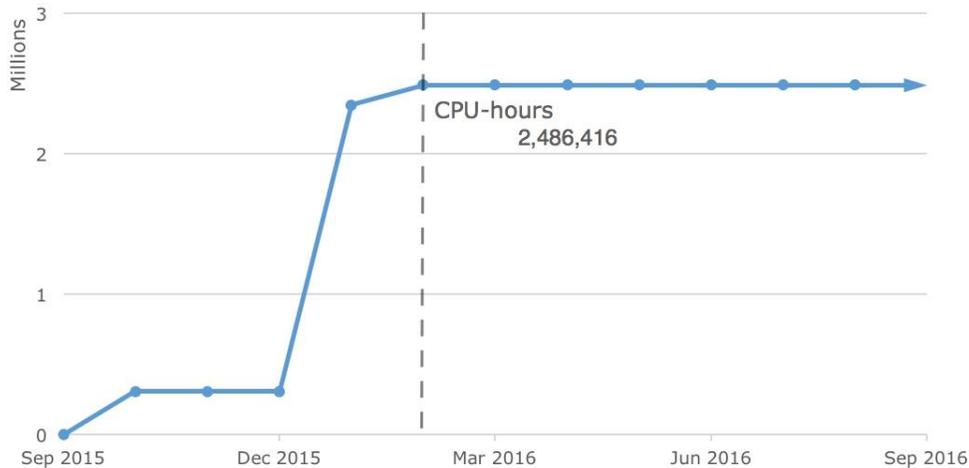
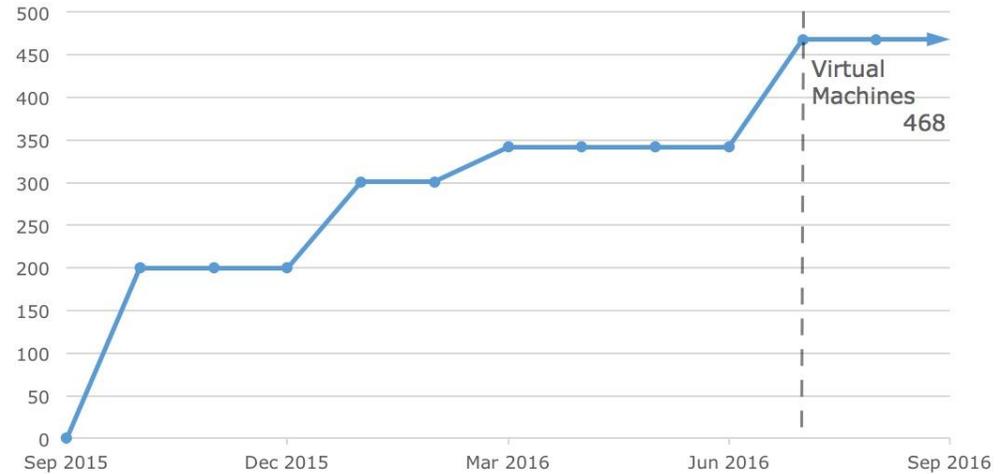
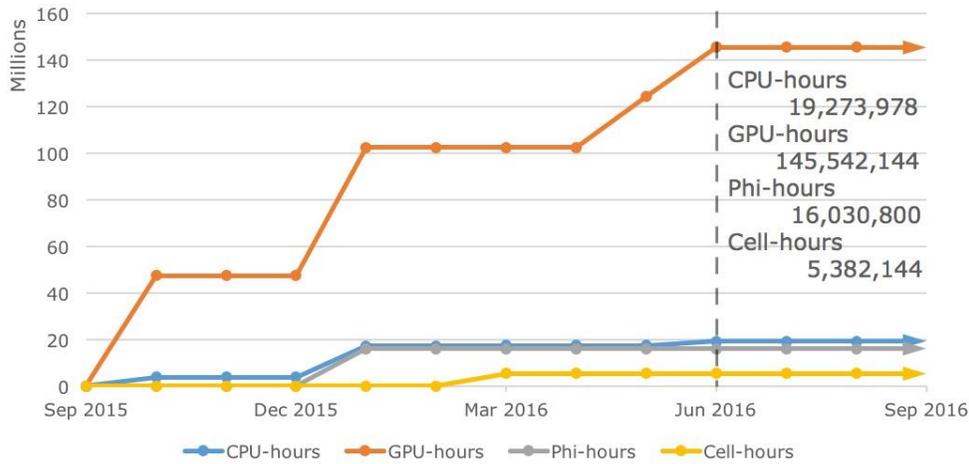
VI-SEEM Storage Resources



Storage resources (KPI: 11,000 TBs)

Resource	Country	Total		Dedicated	
		Disk [TB]	Tape [TB]	Disk [TB]	Tape [TB]
ARIS	Greece	1,000	3,000	50	210
Cyprus	Cy-Tera	500	-	100	-
Avitohol	Bulgaria	96	-	5	-
PARADOX	Serbia	96	-	5	-
NIIFI HSM	Hungary	87	6,800	3	300
NIIFI iSCSI	Hungary	1,000	-	50	-
UVT HPC GPFS	Romania	50	-	5	-
ETFBL-CC01	BIH	1	-	0.5	-
MK-04-FINKI	FYROM	36	-	2	-
RENAMstor	Moldova	4	-	1	-
IIAP Storage	Armenia	8	-	3	-
BA-IA	Egypt	5,200	-	100	-
IUCC Storage	Israel	40	-	5	-
Total		8,118	9,800	329.5	510

Overview of Available Resources



Overview of services deployed – registered in VI-SEEM GOCDB.



GOCDB 5.5

- Browse
 - My Sites
 - Projects
 - NGIs
 - Sites
 - Service Groups
 - Services
- Add
 - Add Site
 - Add Service Group
 - Add Service
 - Add Downtime
- Downtimes
 - Active & Imminent
- About GOCDDBS
 - Role Action Map
 - Doc, Help & Support

Search

Submit

User Status

Unregistered user

Register

Retrieve Old Account

GOCDDB is an EGI service provided by STFC co-funded by EGI.eu and EGI-Engage

Welcome to GOCDDB

GOCDDB is the official repository for storing and presenting EGI topology and resources information.

What information is stored here?

The GOCDDB data consists mainly of:

- Participating National Grid Initiatives (NGI)
- Grid Sites providing resources to the infrastructure
- Resources and services, including maintenance plans for these resources
- Participating people, and their roles within EGI operations

Data are provided and updated by participating NGIs, and are presented through this web portal.

Please note:

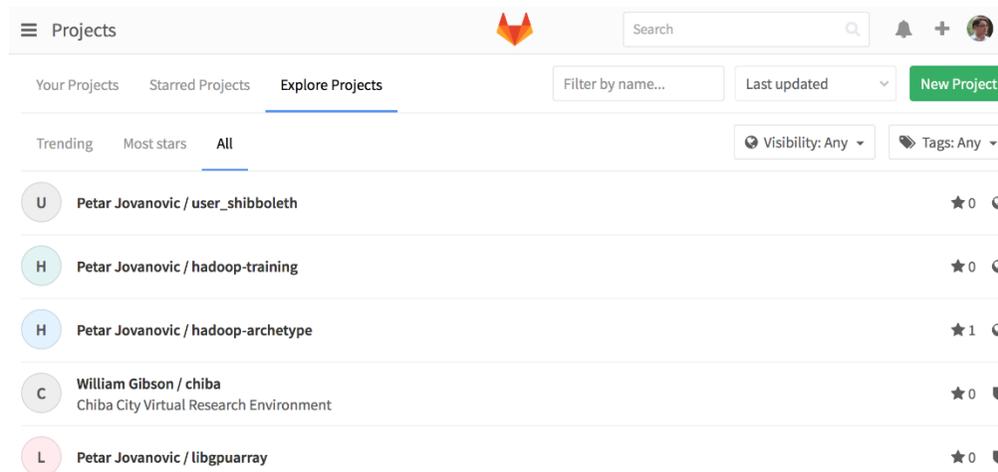
- It is a "catch-all" service. This means if it is centrally hosted on behalf of all NGIs.
- If an organisation deploys and uses their own system or a local GOCDDB installation, their data won't appear here.



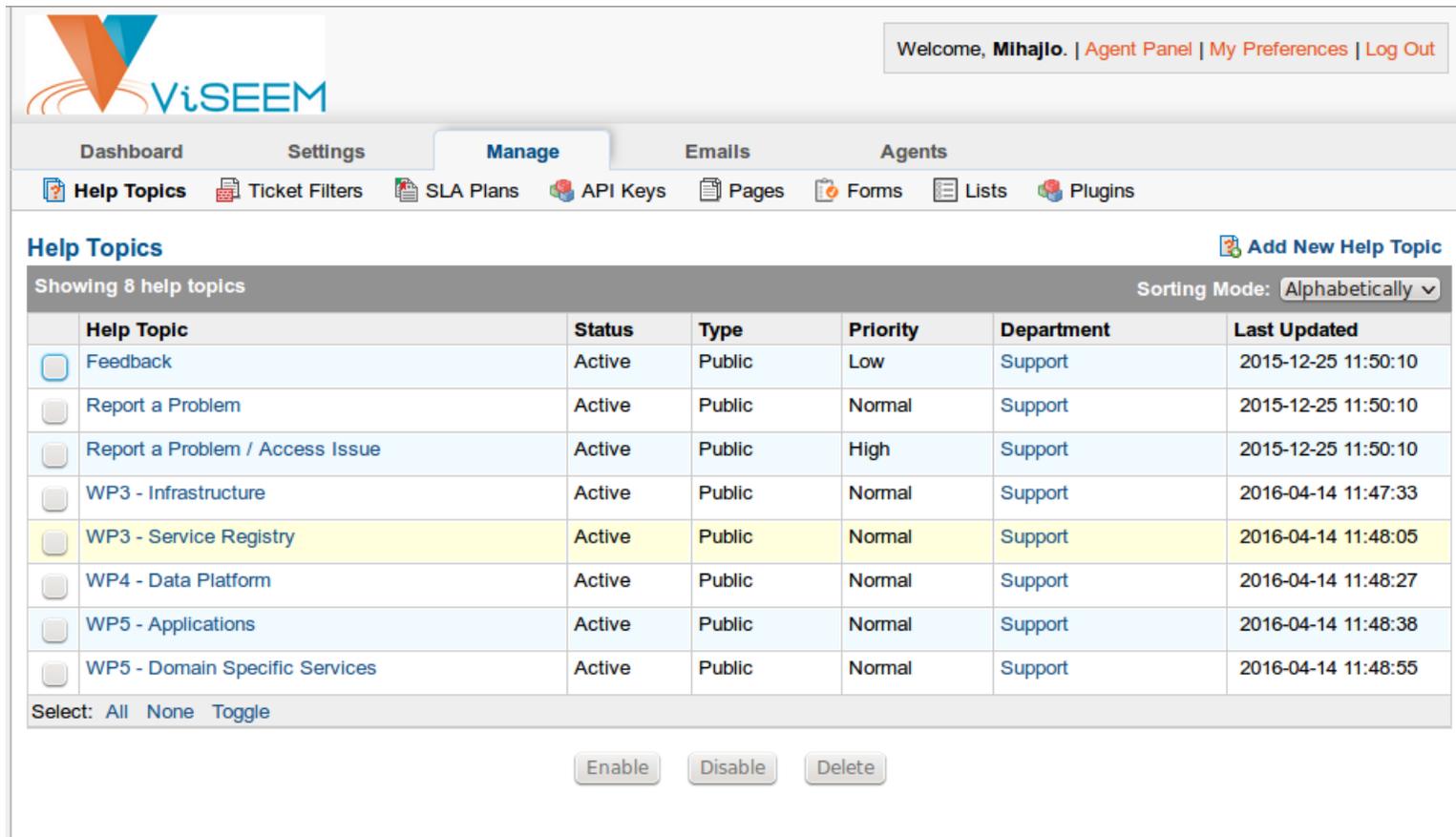
Source Code Repository



- ❑ Deployed at UoBL, GitLab-based, <https://code.vi-seem.eu/>
- ❑ Fully integrated with project's AAI – VI-SEEM Login service and documented at VI-SEEM wiki
[http://wiki.vi-seem.eu/index.php/Source Code Repository](http://wiki.vi-seem.eu/index.php/Source_Code_Repository)
- ❑ Backup instance deployed at UoM



- Deployed at UoBL, osTicket-based, <https://support.vi-seem.eu/>



The screenshot shows the Vi-SEEM Helpdesk management interface. At the top, there is a navigation bar with tabs for Dashboard, Settings, Manage (selected), Emails, and Agents. Below this is a secondary navigation bar with icons for Help Topics, Ticket Filters, SLA Plans, API Keys, Pages, Forms, Lists, and Plugins. The main content area is titled "Help Topics" and includes a sub-header "Showing 8 help topics" and a "Sorting Mode: Alphabetically" dropdown. A table lists the help topics with columns for Help Topic, Status, Type, Priority, Department, and Last Updated. The "WP3 - Service Registry" row is highlighted in yellow. Below the table are "Select: All None Toggle" and "Enable", "Disable", "Delete" buttons.

Welcome, **Mihajlo**. | [Agent Panel](#) | [My Preferences](#) | [Log Out](#)

Dashboard Settings **Manage** Emails Agents

[Help Topics](#) [Ticket Filters](#) [SLA Plans](#) [API Keys](#) [Pages](#) [Forms](#) [Lists](#) [Plugins](#)

Help Topics

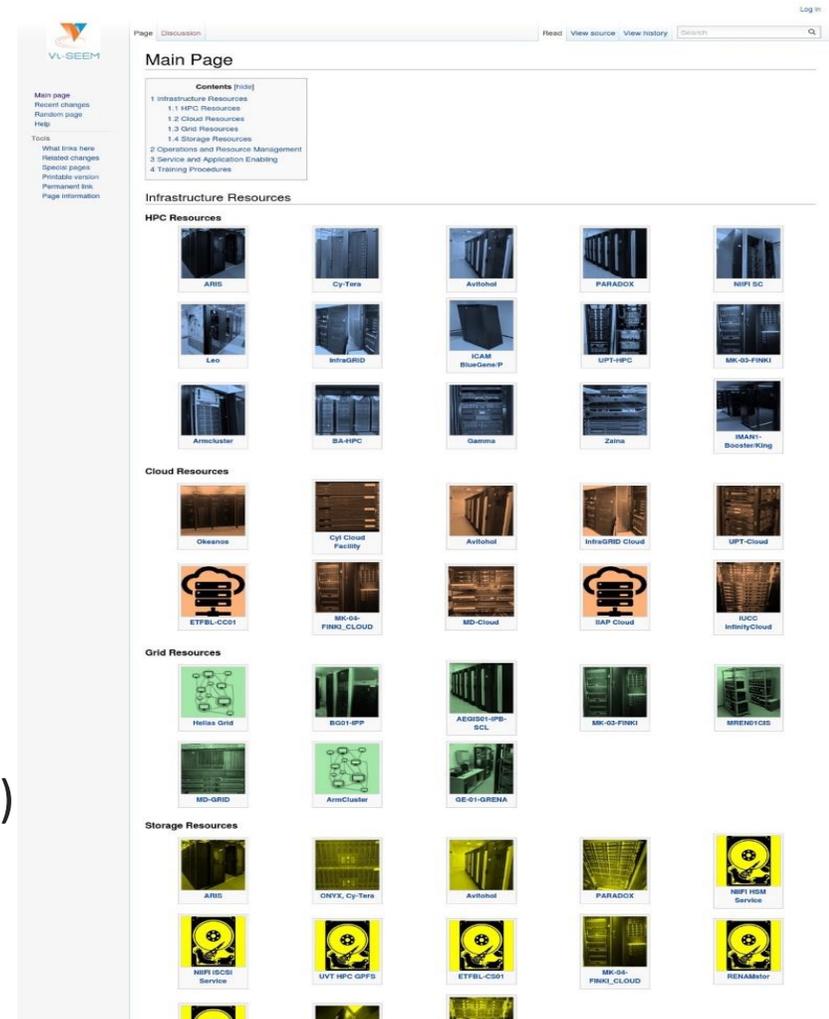
[Add New Help Topic](#)

Showing 8 help topics Sorting Mode: Alphabetically ▾

	Help Topic	Status	Type	Priority	Department	Last Updated
<input type="checkbox"/>	Feedback	Active	Public	Low	Support	2015-12-25 11:50:10
<input type="checkbox"/>	Report a Problem	Active	Public	Normal	Support	2015-12-25 11:50:10
<input type="checkbox"/>	Report a Problem / Access Issue	Active	Public	High	Support	2015-12-25 11:50:10
<input type="checkbox"/>	WP3 - Infrastructure	Active	Public	Normal	Support	2016-04-14 11:47:33
<input type="checkbox"/>	WP3 - Service Registry	Active	Public	Normal	Support	2016-04-14 11:48:05
<input type="checkbox"/>	WP4 - Data Platform	Active	Public	Normal	Support	2016-04-14 11:48:27
<input type="checkbox"/>	WP5 - Applications	Active	Public	Normal	Support	2016-04-14 11:48:38
<input type="checkbox"/>	WP5 - Domain Specific Services	Active	Public	Normal	Support	2016-04-14 11:48:55

Select: All None Toggle

- ❑ Deployed at CYI, MediaWiki-based <https://wiki.vi-seem.eu/>
- ❑ WP3 Wiki documentation
 - ❑ Infrastructure resource (HPC/Grid/Cloud)
 - ❑ Access to resources (HPC/Grid/Cloud)
 - ❑ Source Code Repository User Guide
 - ❑ Support Ticket System User Guide
 - ❑ Source Code Repository User Guide
 - ❑ Supporting vo.vi-seem.eu VO
 - ❑ VI-SEEM Login integration guide (Community Managers and Service Providers)



Monitoring System



- ❑ VI-SEEM monitoring is ARGO-based
- ❑ ARGO POEM service is deployed for VI-SEEM
- ❑ User Interface deployed by UoBL, <https://mon.vi-seem.eu/>

Service Status - All Services

Critical - Community Status of Services

● BA-HPC	● CYI	● GE-01-GRENA
● GRNET	● IIAP-NAS-RA	● IICT-BAS
● IPB	● NIIF	● UKIM
● B2SHARE_GRNET	● B2SHARE_IPB	● B2SHARE_UKIM
● B2SHARE_UVT	● B2STAGE_GRNET	● B2STAGE_IPB

Availability and Reliability - All Services

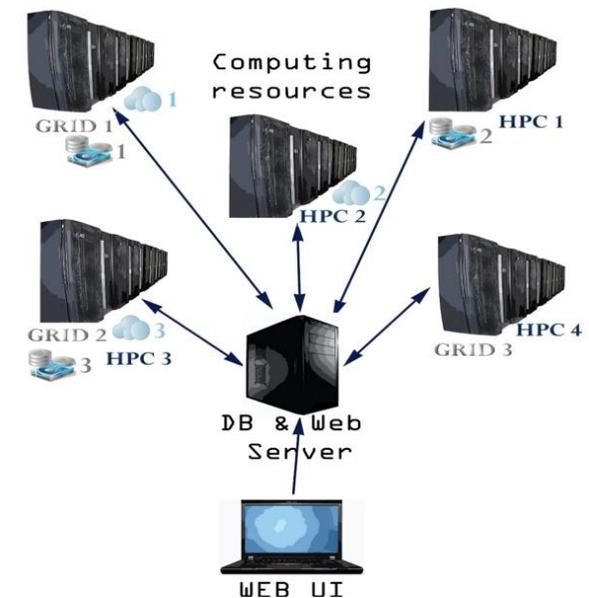
Overall Availability and Reliability Results

Search for a service

Service	2016-09		2016-08		2016-07	
	Availability	Reliability	Availability	Reliability	Availability	Reliability
BA-HPC	94%	94%	0%	0%	0%	0%
CYI	100%	100%	99%	99%	100%	100%
GE-01-GRENA	100%	100%	100%	100%	100%	100%
GRNET	48%	48%	0%	0%	0%	0%
IIAP-NAS-RA	94%	94%	0%	0%	0%	0%
IICT-BAS	100%	100%	98%	98%	99%	99%
IPB	31%	31%	0%	0%	0%	0%

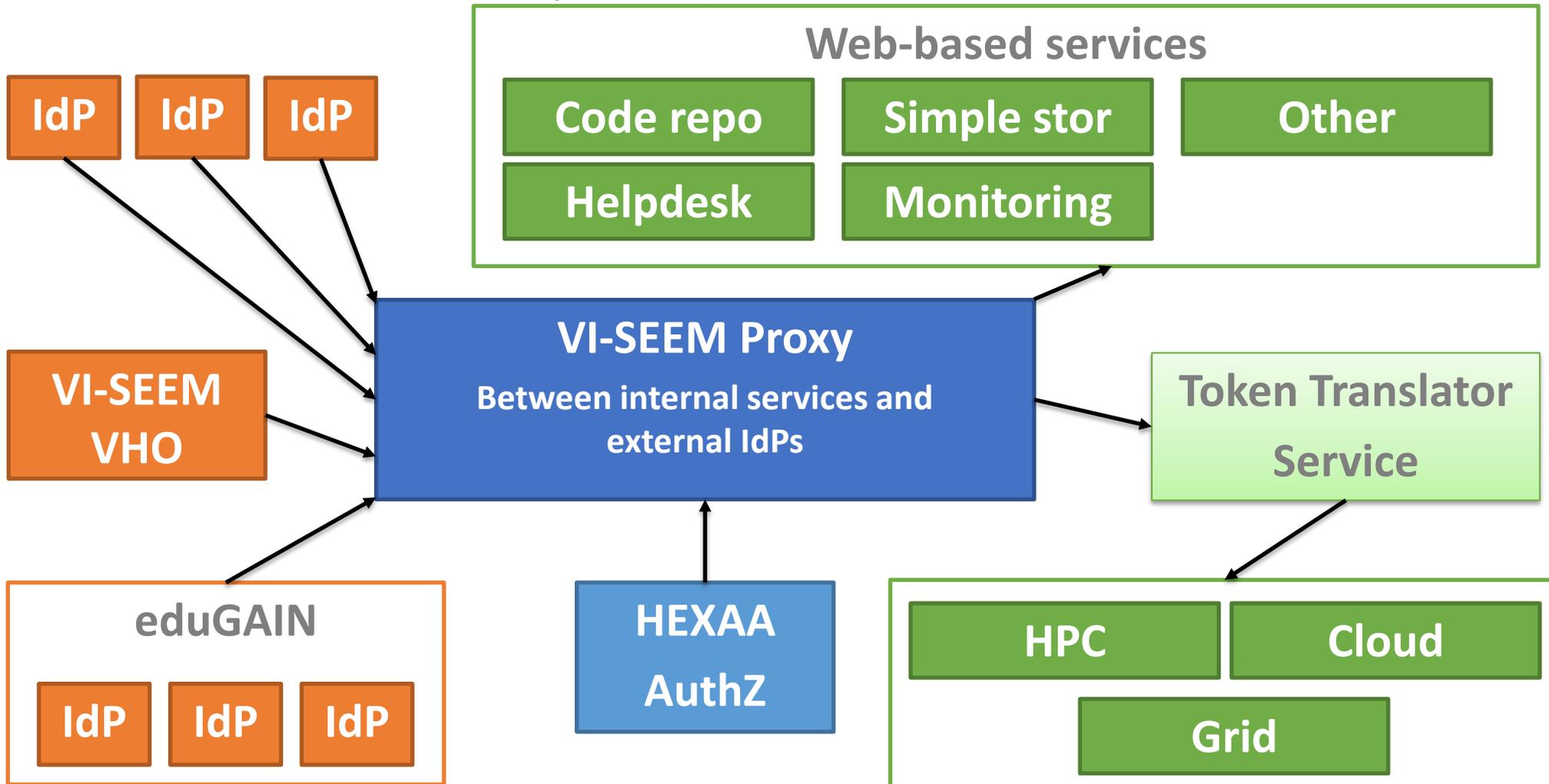
Accounting System

- ❑ Developed at IICT-BAS
- ❑ Provides accurate measurements of the utilization of the different types of resources
- ❑ Client side has accounting publisher packages
- ❑ Publisher will format data into messages and transfer them via AMQP
- ❑ Server side transforms the messages into SQL queries
- ❑ Accounting data will be provided through a web interface
- ❑ Accounting system integrated with the project's AAI
- ❑ Metrics for:
 - ❑ Generic services
 - ❑ Application services



Authentication and Authorization Infrastructure

- Secure, distributed, easy to use, standards-based



- ❑ **VSS – Simple Storage Service** (*simplestorage.vi-seem.eu*)
- ❑ **VRS – Repository Service** (*repo.vi-seem.eu*)
- ❑ **VAS – Archival Service** (*deployed at 4 sites – GRNET, IPB, IICT-BAS, NIIF*)
- ❑ **VLS – work storage space / local storage and data staging** (*at 12 sites*)
- ❑ **VDDS – Data Discovery Service** (*dds.avitohol.acad.bg*)
- ❑ **VDAS – Data Analysis Service** (*hadoop.ipb.ac.rs*)

Virtual research environment and portal content for climate-related research



VRE Portal Up and Running

Content relevant to the Climate Community:

- ❑ **Scientific application environment:**
 - ❑ Optimized applications and libraries for Climate Community
 - ❑ List of supported codes
- ❑ **Regional Community Datasets:**
 - ❑ List of Regional Climate Datasets
- ❑ **Application-Level Services for the regional communities:**
 - ❑ Live Access Server

Live Access Server (LAS)



- ❑ **LAS up and running** on local server at Cyl: las.vi-seem.eu
- ❑ **Rich Initial content**
 - ❑ Feature datasets from global data repositories
 - ❑ Include regional data readily available
- ❑ LAS Implementation **workflow** added to VRE
- ❑ LAS tutorial added to Training Portal
- ❑ Allow **remote data hosting & access**:
 - ❑ Aim to allow individual sites to host data
 - ❑ Individual partners can run interconnected LAS or just serve data through open protocols
 - ❑ LAS Virtual Machine Image produced to be made available on VRE

Digital Cultural Heritage applications

Application Acronym	Country	Responsible Partner	Institute	Scientific Contact
BVL	Romania	UVT	Central University Library "Eugen Todoran" Timisoara	Delia Pârșan
Dioptra	Cyprus	CYI	The Cyprus Institute	Georgios Artopoulos
3DINV	Greece	GRNET	Foundation for Research & Technology, Lab of Geophysical Satellite Remote Sensing and Archaeoenvironment	Nikos Papadopoulos
AutoGR	Greece	GRNET	Institute for Mediterranean Studies Foundation for Research and Technology	Gianluca Cantoro
CH-CBIR	Bosnia and Herzegovina	UNI BL	University of Banja Luka Faculty of Electrical Engineering	Vladimir Risojević
Manuscript	Israel	IUCC	Ben-Gurion University of the Negev	Jihad El-Sana
VirMuf	Egypt	BA	Bibliotheca Alexandrina, International School For Information Science	Mohammed Elfarargy
CHERE	Bosnia and Herzegovina	UNI BL	University of Banja Luka, Faculty of Electrical Engineering	Mihajlo Savic
CSAD	Cyprus	CYI	Centre for the Study of Ancient Documents, Oxford University	Kyriakos Savvopoulos
ELKA	Cyprus	CYI	Ca Foscari Venice	Matthias Kappler
IMC4CH	Bulgaria	NHM	IICT-BAS	Ivan Georgiev and Ivan Hristov
PETRA	Jordan	SESAME	Technical University Berlin, Department of Optics and Atomic Physics	Maram Na'es

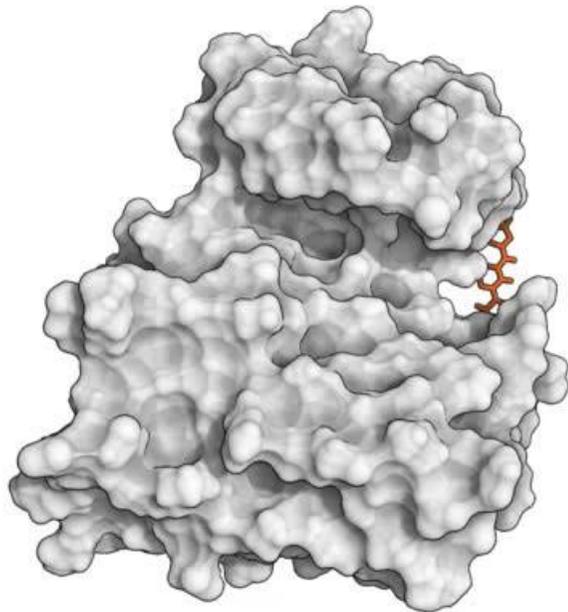
- ❑ **VI-SEEM scientific application environment:** Provides several modules such as optimized applications and libraries, VM images and list of codes, relevant for the work of the regional scientific communities of interest.
- ❑ **Workflow, pipeline and software tools repository:** Provides several modules such as documents containing best practice procedures and workflows for the production of scientific results relevant to the application categories identified in the SEEM region.
- ❑ **Regional Community Datasets:** Provides datasets of regional importance for the scientific communities of interest.
- ❑ **Application-Level Services for the regional communities:** Contains Web-based or visualization services providing easy access to underlying workflows, applications, and resources.
- ❑ **Training Material:** Contains training documentation for several LS areas

VI-SEEM Application Environment

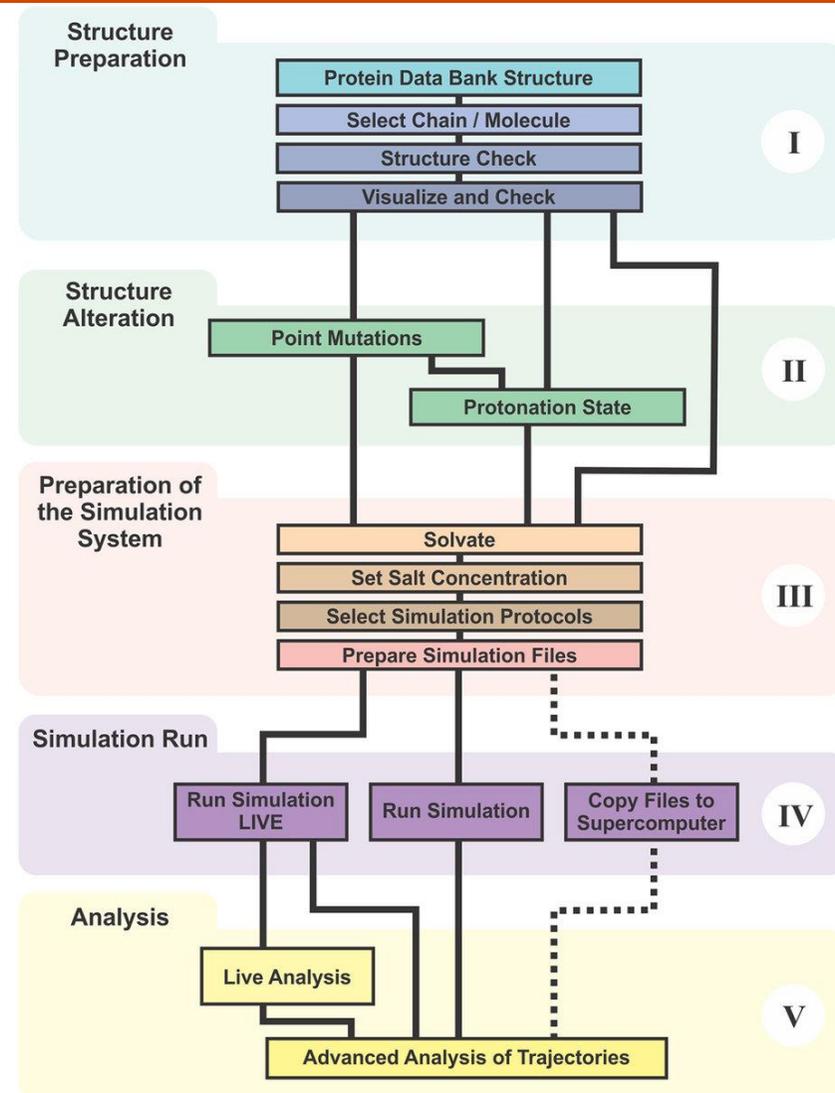


- ❑ Power users obtain access to VI-SEEM HPC facilities with pre-installed development and application software, e.g.:
 - ❑ Intel Parallel Studio XE 2016
 - ❑ GNU Compiler Collection
 - ❑ SPRNG
 - ❑ WRF
 - ❑ OpenFOAM
 - ❑ PETSC
 - ❑ SCALASCA
 - ❑ Etc.
- ❑ More information about Avitohol can be obtained from <http://www.hpc.acad.bg>
- ❑ Contact: **avitohol-support** at parallel.bas.bg

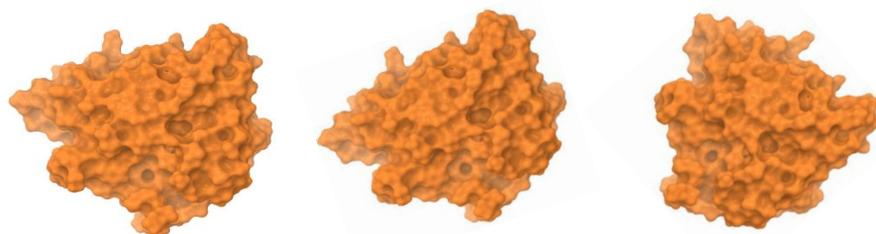
Automating Workflows in VI-SEEM: Molecular Dynamics Simulations



Shan et al (2011)
Cancer drug dasatinib
binding on Src kinase



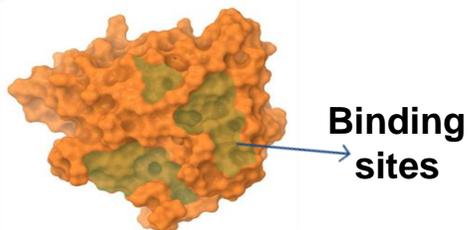
Automating Workflows in VI-SEEM: Virtual Screening for Drug Discovery



Protein conformational Ensemble
Protein Preparation

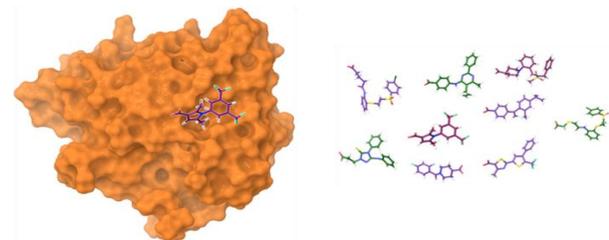


Binding site
identification algorithm

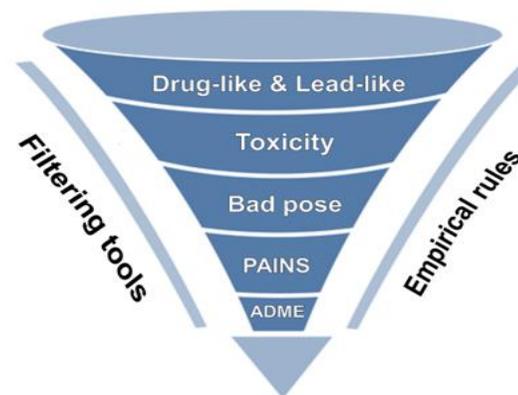


Binding Site implication in large scale
motions (PCA)

Docking & Scoring of
compound libraries



Virtual Screening
algorithm



Compound selection & *in vitro* assays



- ❑ VI-SEEM provides a rich platform for scientific research, encompassing hardware resources, services and support
- ❑ Bulgaria strongly participates in the provisioning and possesses advanced hardware and software infrastructure