VRE for regional communities in Southeast Europe and the Eastern Mediterranean

“Cross-continent collaboration for advanced research”
UbuntuNet-Connect 2017

Dr. Ognjen Prnjat
**Administrative details**

- **VI-SEEM**: Virtual Research Environment for regional interdisciplinary communities in Southeast Europe and the Eastern Mediterranean  
  - Start date 01/10/2015  
  - Duration 36 months

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<th>Participant no.</th>
<th>Participant organisation name</th>
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<th>Country</th>
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<td>SYNCHROTRON-LIGHT FOR EXPERIMENTAL SCIENCE AND APPLICATIONS IN THE MIDDLE EAST</td>
<td>SESAME</td>
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A continuing, integrative effort

- e-Infrastructure built over the last decade
- Targeting less developed EU countries, countries on path to accession and ENP
- Merging of SEE and EM regions
- SEE: network SEEREN1-2, Grid SEE-GRID-1/2/SCI, HPC HP-SEE
- EM: HPC LinkSCEEM1-2
- Cross-continent collaboration!
- Underlying connections via GEANT, ASREN, EaPConnect
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.

- Value added services on top of network
  - Diverse computing technologies
  - Advent of big data / data services
  - Service orientation
Covering the whole life-cycle of scientific research

CLIMATE
LIFE SCIENCES
DIGITAL CULTURAL HERITAGE

- Manage data
- Provide generic and specific services
- Build capacity & collaborations
- Train and support the communities
- Compute, store & transfer
- Enable world-class research
Service catalogue provides service discovery and contains all project services
- Common services and resources operated by WP3
- Storage/data services operated by WP4
- Application-level services provided by WP5
- Designed to be compatible with the FitSM standards
- [https://services.vi-seem.eu/](https://services.vi-seem.eu/)
- 19 services grouped in 5 categories
e-Infrastructure services

- Project e-Infrastructure
  - HPC sites – clusters and supercomputers (different hardware architectures)
  - Grid sites – interconnected via Grid middleware
  - Cloud sites – virtual machines (VMs) for services and distributed computing
  - Storage sites – short and long term storage

- Modern, state-of-the-art technologies for computing, virtualization and storage are made available to the scientific communities

- Overall infrastructure capacity
  - 23,744 CPU-cores, 1,012,736 GPU-cores, 20,496 Xeon Phi-cores
  - 3,112 Grid CPU-cores
  - 14,152 Cloud VM-cores
  - 18 PB of storage space
e-Infrastructure example - HPC sites
e-Infrastructure operations and resource management – collaborative effort

Code Repository, UoBL
https://code.viseem.eu/

Helpdesk, UoBL
https://support.vi-seem.eu/

Accounting, IICT-BAS
https://accounting.vi-seem.eu/

GOCDB, UKIM
https://gocdb.vi-seem.eu/

Monitoring, GRNET/UoBL
https://mon.vi-seem.eu/

Technical Wiki, CYI
https://wiki.vi-seem.eu/
Functions allowing for data management for selected Scientific Communities, engage the full data management lifecycle

- **VSS** – Simple Storage Service (simplestorage.vi-seem.eu)
- **VRS** – Repository Service (repo.vi-seem.eu); integrated with PID service
- **VAS** – Archival Service (deployed at 6 sites – GRNET, IPB, IICT-BAS, NIIF, IUCC, BA)
- **VLS** – work storage space / local storage and data staging (at 12 sites)
- **VDDS** – Data Discovery Service (search.vi-seem.eu)
- **VDAS** – Data Analysis Service (hadoop.ipb.ac.rs)
- **PIDs** (handle.grnet.gr)
Data management services – spread
All services integrated through the user-facing VRE portal

https://vre.vi-seem.eu/

Organized per Scientific Community
- Climate SC
- Life Sciences SC
- Digital Cultural Heritage SC

Access to VI-SEEM services and resources: Compute, Data, Domain-specific, Training

Guidelines on how to contribute to
- Applications
- Workflows/codes
- Datasets
- Domain-specific services

Domain-specific services integrated in the portal in a series of phases carried out by services enablers and user communities
Domain-specific services

- **VRE Scientific Application Environment**
  - Optimized applications and libraries
  - Virtual Machine (VM) images
  - Codes from the three scientific communities

- **Workflow, software tools repository**

- **Regional community datasets**

- **Application level services**
  - **Climate**
    - Live Access Server
  - **Digital Cultural Heritage**
    - VI-SEEM Clowder
    - 3DINV
    - AUTOGR
  - **Life Sciences**
    - ChemBioServer
    - AFMM
    - NANO-Crystal
    - Subtract
Application-level service flagships

- Climate
  - Live Access Server

- Digital Cultural Heritage
  - VI-SEEM Clowder

- Life Sciences
  - ChemBioServer
Live Access Server

http://las.vi-seem.eu/las

A web server providing flexible access to geo-referenced scientific data, offering visualization & post-processing capabilities for climate data
VI-SEEM Clowder

http://dchrepo.vi-seem.eu/

A Digital Culture Heritage repository which also offers integrated interactive visualization tools
ChemBioServer

http://bioserver-3.bioacademy.gr
/Bioserver/ChemBioServer/

A web-based pipeline for filtering, clustering and visualization of chemical compounds used in drug discovery
Access to the VRE

- Defined the framework for accessing VI-SEEM services and resources
- Opened up the VRE to the widest possible regional communities
- Uses a fair, transparent and trusted mechanism for allocation of VRE resources
- Facilitates access and deployment of new applications in the VRE
- 3 calls envisaged
- 40+ applications have been allocated resources
- Scientific support also provided
Access to the VRE - application areas

- Modeling and Molecular Dynamics (MD) study of important drug targets
- Computer-aided drug design
- Analysis of Next Generation DNA sequencing data
- Synchrotron data analysis
- Image processing for biological applications

- Regional climate modelling to better understand and predict climate change and impacts, and phenomena such as dust storms.
- Air quality modelling, including atmospheric chemistry and air pollution transport.
- Weather forecast and extreme weather prediction, model development, application.

- Online services and access to repositories in order to enable studies of the immense cultural heritage assets in the region (e.g., searchable digital libraries; with support of meta-data and OCR for Latin characters).
- Online visualization tools and data management systems to drive breakthrough contributions to art historical problems (e.g., interactive visualization viewer of RTi files and 3D models with digital libraries integration).
- Unsupervised feature learning in photogrammetric techniques, data processing for image classification; semantic referencing; and geo-referencing.
23 project applications, 21 accepted
- 11 in Climatology
- 5 in Digital Cultural Heritage
- 5 in Life Sciences

10 different countries of the region
14 of the applications required HPC services
6 required Grid and Cloud services
12 required storage services
8 required application specific services

Per-country distribution: Bosnia and Herzegovina: 1, Bulgaria: 6, Cyprus: 3, FYR of Macedonia: 2, Georgia: 1, Greece: 4, Montenegro: 1, Israel: 1, Romania: 1, Serbia: 1.

14M CPU core hours, 3.4M GPU core hours, 1M Phi core hours provided
2nd Open call

- Call Opened in May 2017 with deadline June 2017
- 14 Services made available to users
- In total 15 million CPU core hours, 370 million GPU core hours and 15 million Phi core hours are available
- Targeted research fields
  - 5 areas in Life Sciences
  - 3 areas in Climate Research
  - 3 areas in Digital Cultural Heritage
- 18 applications have been received
  - 7 in Life Sciences
  - 5 in Climate Research
  - 6 in Digital Cultural Heritage
Training, dissemination, marketing, innovation

- Content-rich platform for communication within the VRE community and beyond
  - Main web page, VRE portal, training portal, wiki
  - Agenda system, document repository system

- VI-SEEM marketing activities
  - Newsletters, popular articles, promotional materials, focused meeting and events for various types of audiences (SMEs, museums, universities, institutes, etc.), seminars and tours for students

- Events organized
  - 7 national dissemination events
  - 7 national training events
  - 3 regional training events

- 26 external events where project presented
- 25 papers
- 9 innovative developments
VI-SEEM Training Portal

Access via: https://training.vi-seem.eu/

- Storage services
- Domain-specific software and tools
  - Climate
  - Digital Cultural Heritage
  - Life Sciences
- HPC
- Cloud
- Data
- Grid
- Scientific visualization
A case study on regional shared value-added services
- A VRE for the scientific user communities in 3 domains
- Integrated platform bringing together computing, data management and domain-specific services
- Services listed in the Service Catalogue and provided through the VRE Portal
- Support the full lifecycle of scientific research
- User-centric view
- Open calls for access, peer review

African community can benefit from this example of common technical and scientific cross-border endeavor

We would like to help Africa-Connect, UbuntuNet and NRENs add value-added services on top of the network

We are supportive of collaborations with African scientists from the target scientific fields.
We cherish our community and want to enlarge it!
Thanks!

https://vi-seem.eu

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