

# Vi-SEEM



VRE FOR REGIONAL INTERDISCIPLINARY  
COMMUNITIES IN SOUTHEAST EUROPE &  
THE EASTERN MEDITERRANEAN

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vi-seem.eu



# Explore



## What is VI-SEEM?

VI-SEEM is a Virtual Research Environment (VRE) for the Scientific Communities of Life Sciences, Climate Science and Digital Cultural Heritage in Southeast Europe and the Eastern Mediterranean.

VI-SEEM unifies the existing regional High-Performance Computing, Cloud and Grid Computing resources, Data Management services, software and tools, as well as application specific on line software services, and delivers to multi-disciplinary communities an integrated platform for high-quality research.

The Virtual Research Environment is supported by the EC through the Horizon 2020 VI-SEEM project.

## Getting access to the VI-SEEM Virtual Research Environment

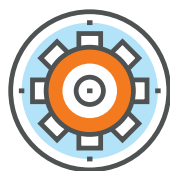
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**ACCESS TO VI-SEEM SERVICES AND RESOURCES IS DESCRIBED AND PROVIDED VIA THE VI-SEEM VRE PORTAL: <https://vre.vi-seem.eu>**

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### Open Access to Datasets

VI-SEEM data services are provided to all users via unrestricted free access (restrictions on fair usage apply), as long as the data sets are accompanied with creative commons or similar license to the users. User registration for statistics purposes applies in some cases.



### Access to VI-SEEM Application Specific Services

Access to the VI-SEEM application specific services, and read access to the code and tools repository is provided for free (user registration might be required) and it is subject to fair usage policy. Development and extension of application-level services is done via the open calls. Users can register to all VI-SEEM services that require registration via the federated VI-SEEM Login service.

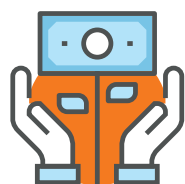
### Access to Computation and Storage Resources

Access to large amounts of computation and storage resources for performing scientific simulations, deploying application-level services, and storing large amounts of data is provided to excellent research projects from the region via the VI-SEEM open calls.

Calls are open once a year, addressed to scientists and researchers that work in academic and research institutions in the region of South Eastern Europe and the Eastern Mediterranean. More specifically these are: Albania, Armenia, Azerbaijan, Bosnia and Herzegovina, Bulgaria, Cyprus, Egypt, FYR of Macedonia, Georgia, Greece, Hungary, Israel, Jordan, Lebanon, Moldova, Montenegro, Romania, Serbia and Turkey.

The proposals undergo a technical review and a lightweight scientific review in order to determine the eligibility and suitability of applications for the requested services and systems. Applications requiring very large amounts of resources that are successful at this stage undergo scientific peer review by independent scientific experts in all countries of the region.

Open calls are advertised via the VI-SEEM website - <https://vi-seem.eu>



### VI-SEEM Access - Contributing to the VRE

Via the open calls applicants are encouraged to extend the range of services VI-SEEM offers, either by contributing to data sets, codes and workflows, or by deploying new application level services. Projects get access to extra resources and user support via the call, while extra support for generating new content or services is given via the VI-SEEM access mechanism.

## User support

<https://tts.vi-seem.eu>  
email: [support@vi-seem.eu](mailto:support@vi-seem.eu)



Our VRE user support team comprises of individuals in all countries of the SEEM region, who run, maintain and administer facilities and services.

We provide to potential users guidance on the services and the requirements to get access to VI-SEEM.

VI-SEEM user support can be offered free of charge to researchers that have gained access to the VI-SEEM services.



## Training offerings

<https://training.vi-seem.eu>

VI-SEEM organizes regional and national training courses to maximize the value of our services for users. Experts from the VI-SEEM scientific communities are providing technical knowledge and advice that enables researchers to get familiar with the benefits of the VRE and how they can use it to cover their high demanding research needs.

The courses consist of basic and specialized topics, followed by hands-on exercises.

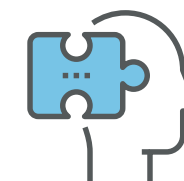
## VI-SEEM training portal

<https://training.vi-seem.eu>

Our training portal collects and curates training material about the VI-SEEM services. It is a focal point of high quality training material and information regarding how to access the VI-SEEM e-infrastructure services (HPC, Grid, Cloud, Data), and how to use the tools, data services and infrastructure available, depending on the scientific field of interest.







# Exploit

## the VI-SEEM Services

<https://services.vi-seem.eu>

The VI-SEEM Service Catalogue offers a broad set of generic as well as application-specific services in the areas of compute resource provisioning, data services provisioning, datasets provisioning, software and scientific workflow provisioning as well as domain-specific applications provisioning.

## Authentication and authorisation: secure access to VI-SEEM e-Infrastructure resources

### VI-SEEM Login

VI-SEEM Login enables researchers to access VI-SEEM e-Infrastructure resources in a user-friendly and secure way, using federated authentication mechanisms. The service also

supports user authentication with social identities, so that users who do not have a federated account at a home organization can seamlessly access the VI-SEEM services without compromising the security of the VI-SEEM infrastructure.

## Compute services: technology for high calibre research

### VI-SEEM HPC Access Service

VI-SEEM HPC enables users to perform complex simulations on state-of-the-art computing hardware, delivering 18.8 CPU, 371.6 GPU, 16.0 Xeon Phi, and 5.3 IBM Cell Millions of core hours per year. It provides access to supercomputers or clusters with low-latency interconnection based on x86\_64 CPUs some of them equipped with accelerator cards, a BlueGene/P system, as well as one Cell processor based system.

### VI-SEEM Cloud Access Service

VI-SEEM Cloud service provides the ability to launch Virtual Machines (VMs) with public/private IPs, and to deploy Virtual Research Environment services for production or backup/fail-over instances. In total 500 VMs or 4 million of VM-hours per year are made available for the target scientific communities.

### VI-SEEM Grid Access Service

VI-SEEM grid provides access to smaller, geographically distributed clusters integrated via Grid middleware. The service enables users to utilize heterogeneous hardware resources using high-capacity approach.

## Data storage services: VI-SEEM solutions for uploading, sharing and retrieving research data

### VI-SEEM Data Discovery Service

<https://search.vi-seem.eu>

VI-SEEM data discovery is a powerful data management system for flexible searching, publishing and sharing of almost any type of data and metadata. The service uses B2FIND technology that is developed in the ongoing EUDAT project (<https://eudat.eu>) and the CKAN open-source platform (<https://ckan.org>).

### VI-SEEM Archival Service

The service offers safe data archiving and automatic replication with high availability and performance. Data archives are indexed and have search capabilities so that files and parts of files can be easily located and retrieved. Archived data are important for future reference and reproducibility of scientific simulations.

### VI-SEEM Simple Storage

<https://simplestorage.vi-seem.eu>

VI-SEEM Simple Storage service allows members of the target scientific communities to keep and sync research data on various devices, as well as to share this data thus making it a useful collaborative tool. Access is enabled via web browsers, desktop and mobile clients.

### VI-SEEM Repository

<https://repo.vi-seem.eu>

VI-SEEM Repository is the main storage service that allows users of the VI-SEEM VRE to deposit and share data, including publications and their associated data, software, references to software and workflows. The service also hosts simplified data formats such as images, videos or others suitable also for the general public.

## Application specific services: domain-specific services for Life Sciences, Climate Science and Digital Cultural Heritage research

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### SERVICES FOR LIFE SCIENCES RESEARCH: A PIPELINE WITH INNOVATIVE TOOLS FOR COMPUTER-AIDED DRUG DESIGN

#### Subtract

<http://subtract.vi-seem.eu>

Subtract is an online tool that can calculate the volume of a binding site found in a protein. It accepts an atom selection and computes the three-dimensional convex hull of the atoms points. The algorithm computes the volume of the convex hull and the volume of the atoms that are included in the solid. The subtraction of those two volumes yields the volume of the investigated cavity. The algorithm computes cavity volumes of trajectory frames in parallel for maximum efficiency and speed.

#### ChemBioServer

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

ChemBioServer is a web-application for effectively mining and filtering chemical compounds used in drug discovery. ChemBioServer allows for pre-processing of compounds, as well as for post-processing of top-ranked molecules resulting from a docking exercise with the aim to increase the efficiency and the quality of compound selection that will pass to the experimental test phase.

## AFMM

<http://afmm.vi-seem.eu>

AFMM provides an automated platform with which the users can generate parameters for modelling small molecules with Molecular Dynamics simulations. The program optimizes an initial parameter set -either pre-existing or using chemically-reasonable estimation, by iteratively changing them until the optimal fit with the reference set is obtained. By implementing a Monte Carlo-like algorithm to vary the parameters, the tedious task of manual parameterization is replaced by an efficient automated procedure.

## NANO-Crystal

<http://nanocrystal.vi-seem.eu>

NANO-Crystal is a web-based tool, for the construction of spherical nanoparticles of a given radius. The goal is to find the number and the

Cartesian coordinates of smaller spheres that fit on the surface of the nanoparticle and visualize the output morphology. The program computes the number of smaller spheres that fit on the bigger surface and the user can download their Cartesian coordinates. The tool is complemented by a crystal computational morphology toolbox for constructing and modelling different crystal nanoparticle shapes.

## DICOM

<http://viseem.dicom.md>

DICOM Network is a service that aids the collection, process and visualization of medical images online. It consists of the DICOM Portal, a front-end user interface for patients, doctors, scientists, the DICOM Server, which collects and archives images to DICOM portal for online access, and the DICOM Viewer for visualization, 3D modelling and medical image editing.

# 2

## SERVICES FOR CLIMATE RESEARCH: FLEXIBLE ACCESS TO GEO-REFERENCED SCIENTIFIC DATA

### VI-SEEM Live Access Server

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

Live access server is a highly configurable server designed to provide flexible access to geo-referenced scientific data. The application enables

the user to visualize data with on-the-fly graphics, request custom subsets of variables in a choice of file formats, access background reference material about the data (metadata), and compare variables from distributed locations.

# 3

## SERVICES FOR DIGITAL CULTURAL HERITAGE RESEARCH: MANAGING COMPLEX REPRESENTATIONS OF DATA

### VI-SEEM Clowder

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

Clowder is a research data management system deployed to support the VI-SEEM digital cultural heritage community by being able

to handle any data format. Clowder provides three major extension points: pre-processing, processing and previewing. Users can upload, download, search, visualize and get various information about cultural heritage data in the region.

## Cross disciplinary services: access to software tools, applications, documentation and training material

### VI-SEEM Workflow and Software Tools Repository

<https://code.vi-seem.eu>

The service provides access to several modules such as documents containing best practice procedures and workflows for the usage of available datasets and codes for the production of scientific results.

### VI-SEEM Regional Community Datasets

<https://repo.vi-seem.eu>

<https://search.vi-seem.eu>

This service provides access and information regarding datasets of regional importance for the scientific communities of interest. Examples of such datasets are the RTi dataset of

ancient Cypriot coinage (Digital Culture Heritage) and Datasets with data for thermodynamic stability of RNA/DNA and DNA/DNA duplexes (Life Sciences). The datasets can be downloaded and used by the customer for research and education purposes.

### VI-SEEM Scientific Application Environment

<https://vre.vi-seem.eu/index.php/scientific-application-environment>

VI-SEEM scientific application environment provides access and information to several optimized software modules such as scientific applications and libraries, virtual machine images and list of codes, relevant for the work of the regional scientific communities.





# Excel



The VRE enables scientists to run research activities of international standing in the fields of Life Sciences, Climate Science, and Digital Cultural Heritage, to address a plethora of scientific and social challenges.



## Life Sciences

Advanced services for understanding disease mechanisms in the populations of the region facilitated by the rich Virtual Research Environment.

- Modelling and Molecular Dynamics study of important drug targets
- Computer-aided drug design, analysis of next generation DNA sequencing data
- Synchrotron data analysis and image processing for biological applications.



## Climate Science

e-Infrastructure resources to predict global and regional climate change, weather extremes, and related impacts.

- Regional climate modelling to better understand and predict climate change and impacts, as well as climatic phenomena such as dust storms



- Air quality modelling, including atmospheric chemistry and air pollution transport
- Model development and application for weather forecast and extreme weather prediction.



**Digital Cultural Heritage**

Sophisticated tools and techniques for new understanding of the past and more accurate interpretations of historical interactions between human actors, agency and the rich heritage of regional cultures.

- Online services and access to repositories for enabling studies of the immense cultural heritage assets in the region, such as searchable digital libraries; with support of metadata 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.

**VI-SEEM CONSORTIUM**

GRNET (Greece)	UPT (Albania)	IIAP-NAS-RA (Armenia)
Cyl (Cyprus)	UNI BL (Bosnia and Herzegovina)	GRENA (Georgia)
IICT-BAS (Bulgaria)	UKIM (FYR of Macedonia)	BA (Egypt)
IPB (Serbia)	UOM (Montenegro)	IUCC (Israel)
KIFU (Hungary)	RENAM (Moldova)	SESAME (Jordan)
UVT (Romania)		



Project acronym: **VI-SEEM**  
Call Identifier: **H2020-EINFRA-2014-2015**  
Type of action: **RIA**  
Start date: **01/10/2015**  
Duration: **36 months**  
Total budget: **3,300,000 €**







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