

# Exploiting the Resources of a University HPC Center

Dana PETCU

# HPC Center infrastructure



2009



2011



2013



# Available infrastructure

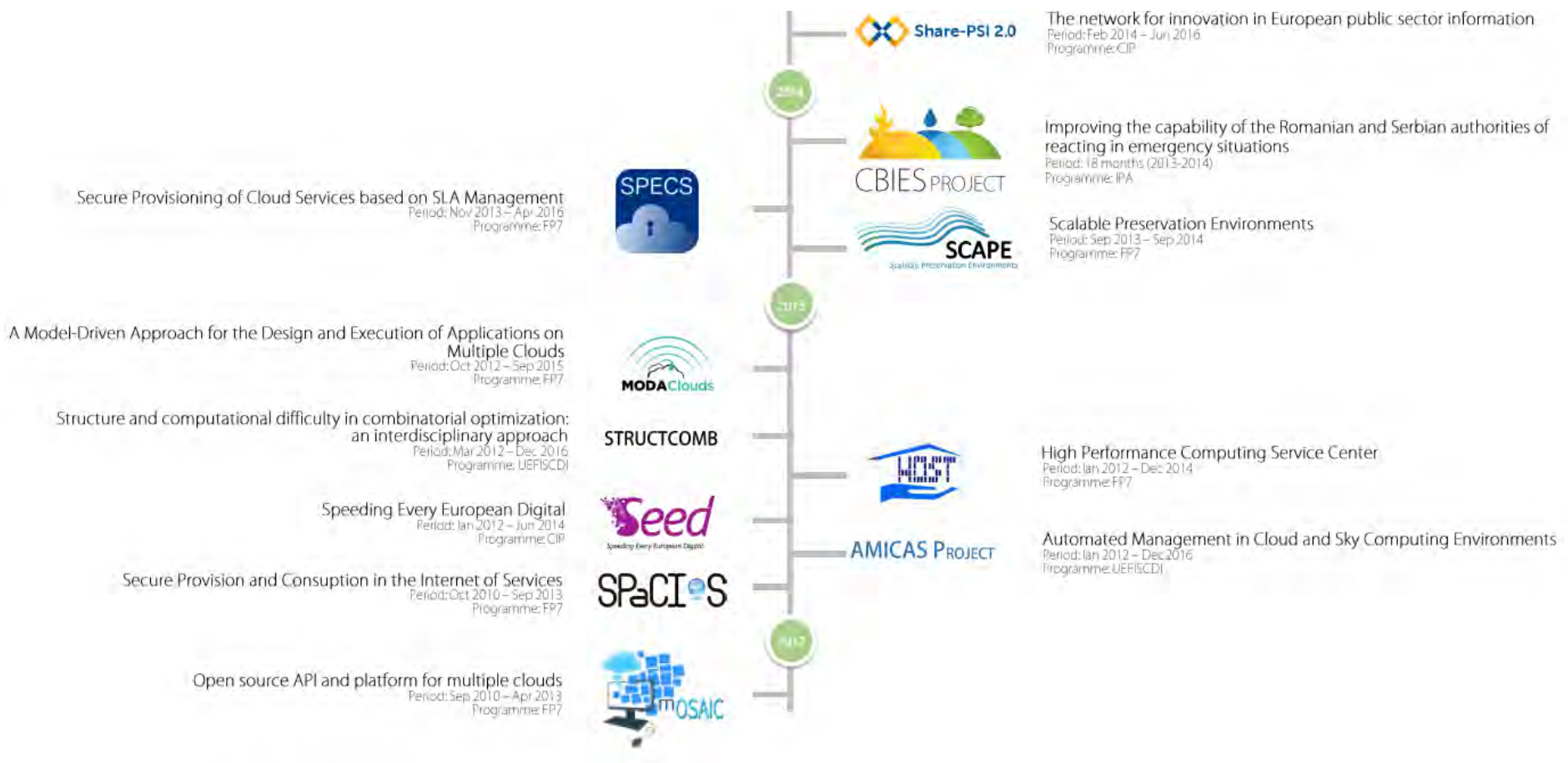


Label	Computing power	Computing units	Internal memory	External memory
[InfraGRID] CPU Cluster	<b>1.5 TFlops</b>	<b>400</b> cores	<b>500</b> GB	<b>13.5</b> TB
[ICAM] BlueGene/P	<b>13</b> TFlops	<b>4096</b> cores	<b>4</b> TB	<b>28</b> TB
[HOST] GPU Cluster	<b>3.6</b> Tflops	3100 CUDA cores	224GB + 42GB (GPU)	16.5 TB
Total :	<b>18 TFlops</b>		<b>4.8 TB</b>	<b>58 TB</b>

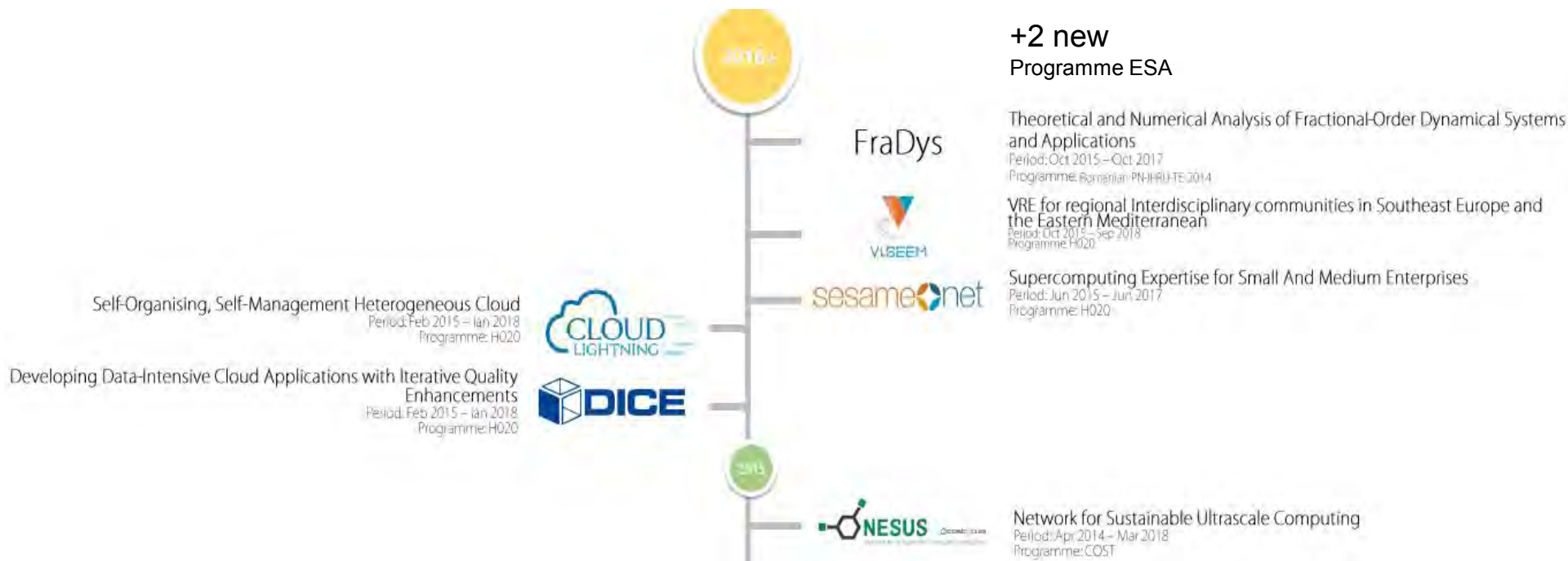
- **UVT, permanent:**
  - Education: Computer Science Department
  - Research: Physics/Geography/CS Deps.
- **Associates, permanent:**
  - Institute e-Austria Timisoara
- **Locals, at request:**
  - Romanian Academy, Timisoara branch
- **National, at request:**
  - PhD students/Researchers
- **European, partners in on-going projects**
  - Researchers, academics, company employers

- **Main topics of research:**
  - HPC
  - Distributed systems
  - AI
- **Organisation:**
  - Researchers in the Center of Research in Informatics of UVT
  - Researchers in Institute e-Austria Timisoara
- **Current positions:**
  - 6 seniors
  - 7 postdocs
  - 10 PhD students + 3 master students
- **Funding:**
  - Based on projects granted through competitions

# Recent projects/CS



# Current projects/CS



## +2 new Programme ESA

Theoretical and Numerical Analysis of Fractional-Order Dynamical Systems and Applications

Period: Oct 2015 – Oct 2017  
Programme: Romanian PN-III-FE-2014

VRE for regional Interdisciplinary communities in Southeast Europe and the Eastern Mediterranean

Period: Oct 2015 – sep 2018  
Programme: H2020

Supercomputing Expertise for Small And Medium Enterprises

Period: Jun 2015 – Jun 2017  
Programme: H2020

Network for Sustainable Ultrascale Computing

Period: Apr 2014 – Mar 2018  
Programme: COST

**VRE for regional Interdisciplinary  
communities in Southeast Europe and  
the Eastern Mediterranean**

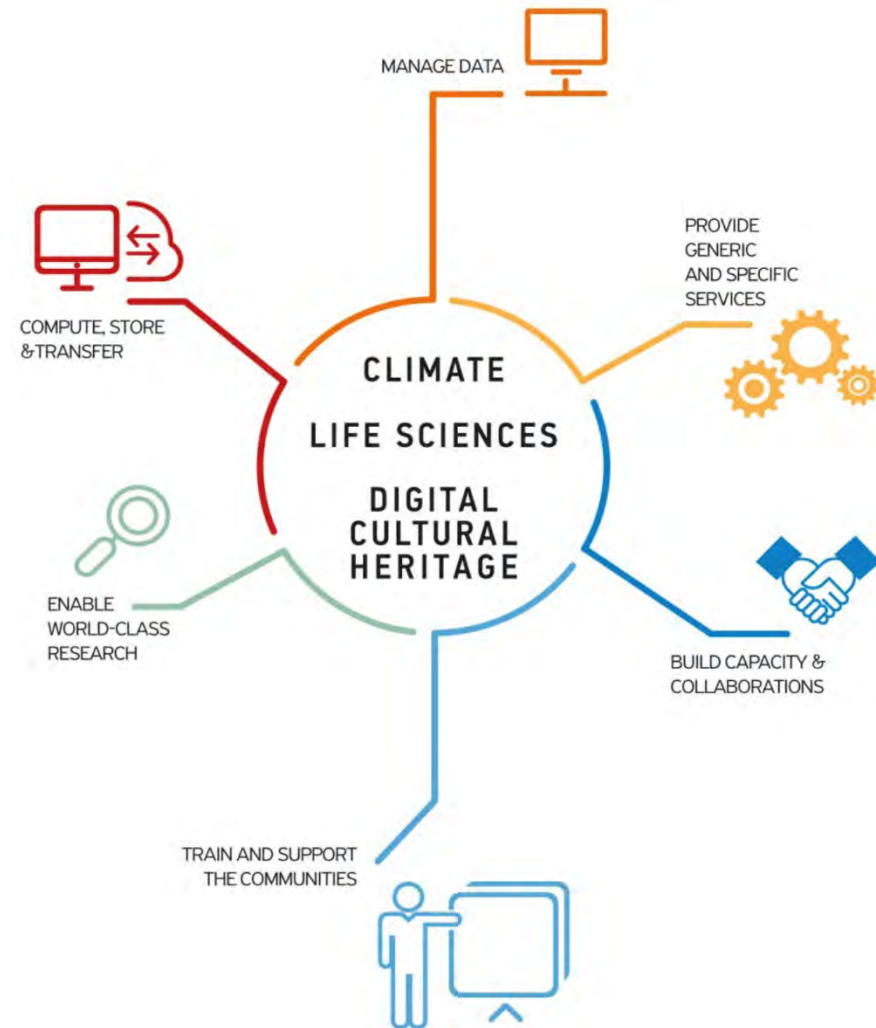
**VI-SEEM Virtual Research  
Environment and Services**





# VI-SEEM VRE and Services

- ❑ 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 Partnership



Greece



Cyprus



Bulgaria



Serbia



Hungary



Romania



Albania



Moldova



FYR of  
Macedonia



Montenegro



Bosnia and  
Herzegovina



Armenia



Georgia



Egypt



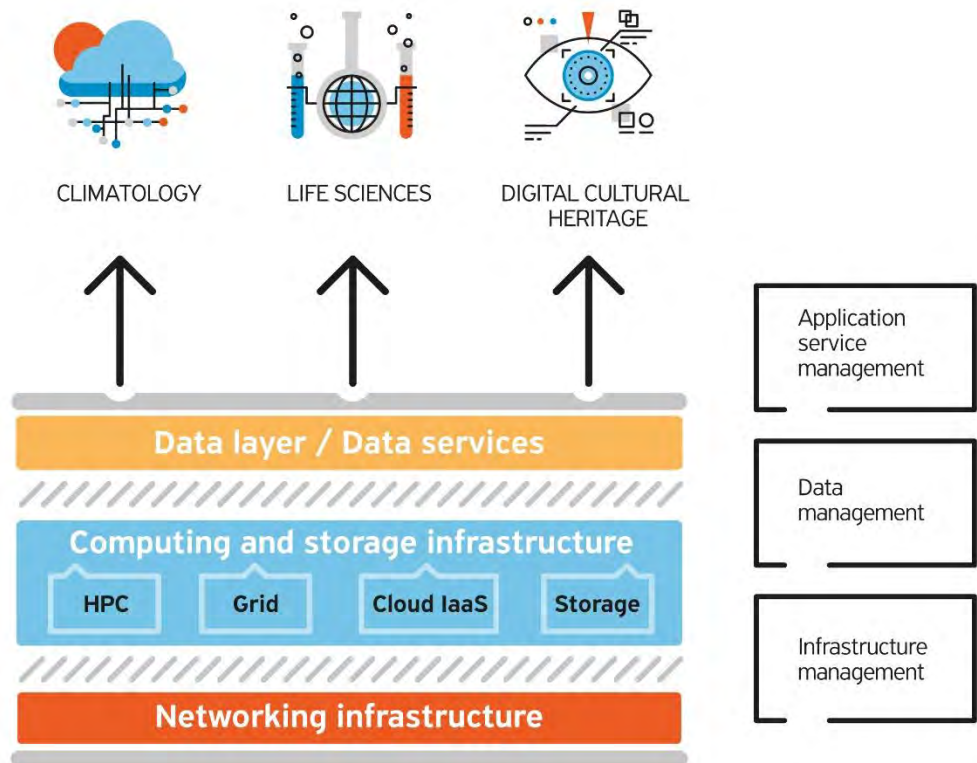
Jordan



Israel

# VI-SEEM VRE and Services

- ❑ Unifies existing e-Infrastructures into an integrated platform
- ❑ Improved service provision within a unified VRE in South East Europe and Eastern Mediterranean
- ❑ Facilitate regional interdisciplinary collaboration
- ❑ Ensure continuity and expansion of the available resources and services



# Objectives

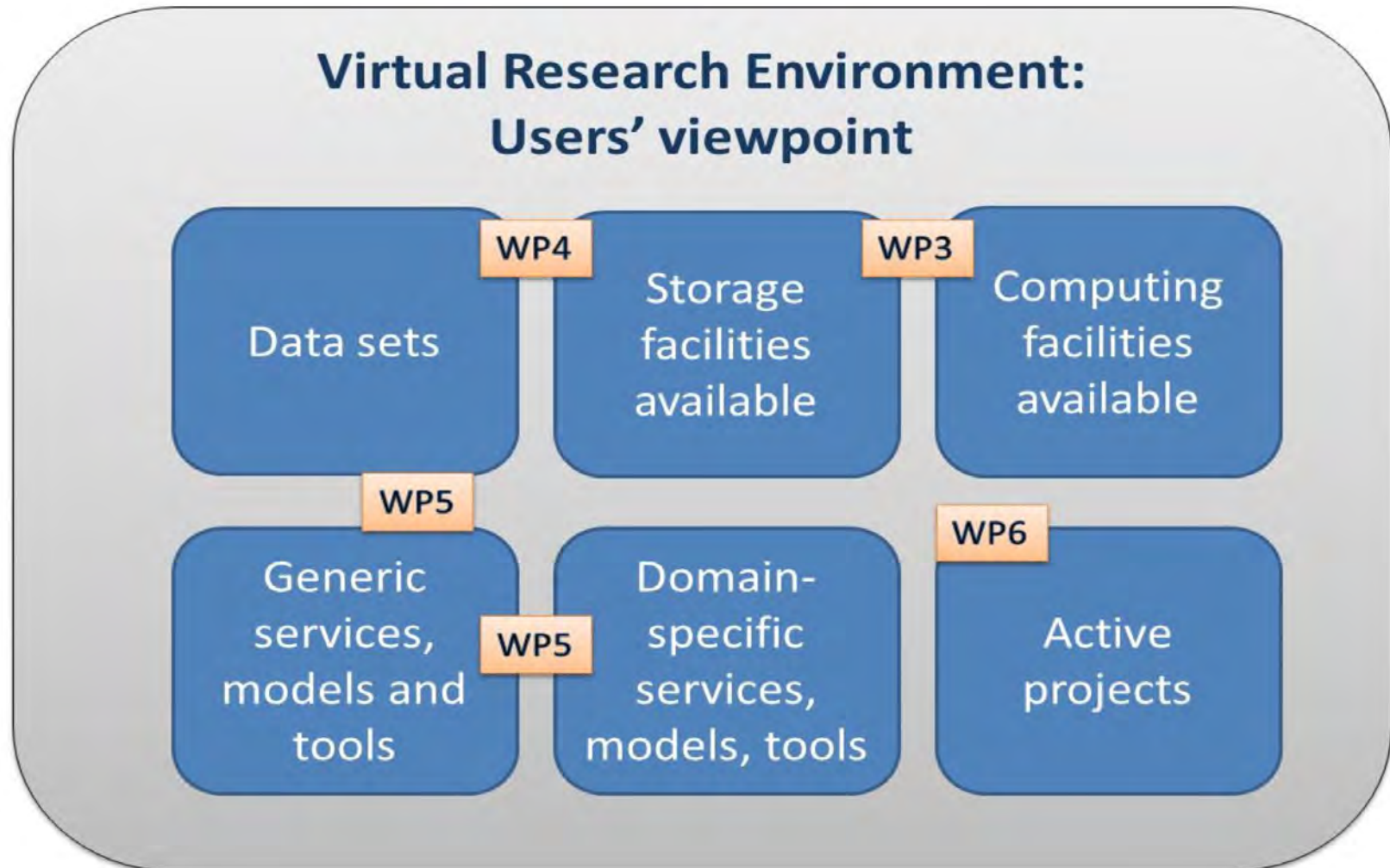


# VI-SEEM Computing Services

- ❑ VI-SEEM HPC service delivers 18.8 million CPU hours, 371.6 million GPU hours, 16.0 million Xeon Phi hours, and 5.3 million IBM Cell CPU hours per year
- ❑ VI-SEEM Cloud service provides the ability to launch VMs with public/private IPs; In total 500 VMs or 4 million of VM-hours per year are made available
- ❑ VI-SEEM Grid service provides access to smaller, geographically distributed clusters integrated via Grid middleware
- ❑ VI-SEEM Storage services deliver 1 PT of storage space.

# VI-SEEM VRE and Services

## Virtual Research Environment: Users' viewpoint



## ❑ Infrastructure

- ❑ Provision of HPC, Cloud and Grid resources (most partners are infrastructure providers)

## ❑ Operational services

### ❑ VI-SEEM Code repository

- ❑ Used to upload source codes produced in the context of the project, or host source code from communities
- ❑ STATUS: Running and integrated with VI-SEEM Login

### ❑ VI-SEEM Service Catalogue

- ❑ Used to provide information about VI-SEEM Services to end users as well as for managing the service portfolio internally
- ❑ STATUS: In production, Integrated with VI-SEEM Login

## □ Services

- VI-SEEM Service instance registry
  - Used to provide information about the deployed service end points
  - STATUS: GOCDB. Deployed. On going addition of services, not integrated with VI-SEEM Login
- VI-SEEM Monitoring: In development (UI)
- VI-SEEM Accounting: In development
- VI-SEEM Login
  - The AAI infrastructure of the project.
  - STATUS: Deployed, Integration with new Identity providers
- TTS:
  - Helpdesk, to be actively used when production applications start using the services
  - STATUS: In production, not integrated with VI-SEEM Login
- VI-SEEM Wiki:
  - Provides the internal (mainly) documentation of the project.
  - Operational not integrated with VI-SEEM Login



- ❑ VI-SEEM Simple Storage
  - ❑ Used to store simple files, important for everyday use and collaboration
  - ❑ STATUS: Available and integrated with VI-SEEM Login
- ❑ VI-SEEM Repository
  - ❑ Used as a generic longer term dataset repository
  - ❑ STATUS: Available and integrated with VI-SEEM Login, need to collect and add datasets
- ❑ VI-SEEM Search
  - ❑ Used to consolidate all data sets (via metadata harvesting) that are available to VI-SEEM
  - ❑ STATUS: Available, needs to integrate metadata with other services (VI-SEEM Repo, Clowder and LAS, and other repos)

- ❑ VI-SEEM Archiving
  - ❑ For safe archiving of large data sets
  - ❑ STATUS: Initial deployment in place. Needs to be formalized and described in service catalogue (will be used via the 1<sup>st</sup> call), VI-SEEM Login integration to be discussed
- ❑ VI-SEEM Work Storage
  - ❑ Used to transfer files among HPC centers for processing in HPC apps
  - ❑ STATUS: Needs to be formalized and described in service catalogue (will be used via the 1<sup>st</sup> call)
- ❑ Data analytics
  - ❑ Used to process data using hadoop
  - ❑ STATUS: Needs to be added to the service catalogue
- ❑ PID Service is also available but not integrated yet with the rest of the services (in progress)

- ❑ VRE Platform
  - ❑ The main entry point for the user communities of the region and beyond
  - ❑ STATUS: Available, To be demonstrated and its structure and content to be discussed
- ❑ Scientific Application Environment
  - ❑ Software modules that are installed and optimized for the use by the communities
  - ❑ STATUS: In production. To be added to the service catalogue.
- ❑ Workflow and Software tools
  - ❑ Used to provide a series of “processes” for scientific simulations
  - ❑ STATUS: Workflows are available as documents, need to identify potential ones for implementation
  - ❑ Identify source codes or Virtual Machines that are suitable for provision to the rest of the community

- ❑ Regional community datasets
  - ❑ Used to share research data sets
  - ❑ STATUS: Some exist and they are stored in different services i.e. Clowder, LAS, VI-SEEM repo, or remote community repositories, need to be integrated with VI-SEEM Search service.
- ❑ Application Level Services
  - ❑ Application specific services
  - ❑ STATUS: Clowder, Live Access Server and ChemBioServer are available. Need to identify new ones and add all of them to the service portfolio

# Example: VI-SEEM Repository

- ❑ The VI-SEEM Repository provides long term data preservation, suitable for data set sharing

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

- ❑ Use cases

- ❑ To store curated data sets for long term preservation
- ❑ To share those datasets with selected collaborators or open them up to whole communities, via web interface
- ❑ To make such data sets searchable by means of associating meta data and then harvesting them
- ❑ Enables scientific communities to capture and describe digital works using a custom submission workflow module

# Benefits of VI-SEEM Repo

## ❑ Some example benefits:

- ❑ Getting your research results out quickly, to a worldwide audience
- ❑ Reaching a worldwide audience through exposure to search engines such as Google
- ❑ Storing reusable teaching materials that you can use with course management systems
- ❑ Archiving and distributing material you would currently put on your personal website
- ❑ Storing examples of students' projects (with the students' permission)
- ❑ Showcasing students' theses (again with permission)
- ❑ Keeping track of your own publications/bibliography
- ❑ Having a persistent network identifier for your work, that never changes or breaks
- ❑ No more page charges for images. You can point to your images' persistent identifiers in your published articles.

# Types of data in the VI-SEEM Repository

- ❑ Articles
- ❑ Preprints, e-prints
- ❑ Technical Reports
- ❑ Working Papers
- ❑ Conference Papers
- ❑ E-theses
- ❑ Audio/Video
- ❑ Lecture notes, Visualizations, simulations
- ❑ Datasets in various formats
  - ❑ Experimental
  - ❑ Simulation
  - ❑ Input
  - ❑ Output
- ❑ Images
- ❑ Visual, scientific
- ❑ Teaching material
- ❑ Digitized library collections



Login

🏠 VI-SEEM Repository Home

## VI-SEEM Repository

Kyriakos says hello. DSpace is a digital service that collects, preserves, and distributes digital material. Repositories are important tools for preserving an organization's legacy; they facilitate digital preservation and scholarly communication.

## Communities in DSpace

Select a community to browse its collections.

VI-SEEM Climate Sciences

The VI-SEEM Climate Sciences Community

VI-SEEM Digital Cultural Heritage

The VI-SEEM Digital Cultural Heritage Community

VI-SEEM Life Sciences

The VI-SEEM Life Sciences Community

VI-SEEM Project Community

The VI-SEEM Project Community

## Recently Added



### BROWSE

All of DSpace

Communities & Collections

By Issue Date

Authors

Titles

Subjects

### MY ACCOUNT

Login

Register

### DISCOVER

Author

Demetroullas, Constantinos (1)

Liketis, Ioannis (4)



## VI-SEEM Climate Sciences

### BROWSE BY

[By Issue Date](#) [Authors](#) [Titles](#) [Subjects](#)

Search within this community and its collections:



Virtual Communities

Climate

The VI-SEEM Climate Sciences Community Repository

2016 The VI-SEEM Climate Sciences Community Repository

### Collections in this community

Test collection

Test collection

Search DSpace

This Collection

### BROWSE

All of DSpace

Communities & Collections

By Issue Date

Authors

Titles

Subjects

This Collection

By Issue Date

Authors

Titles

Subjects

### MY ACCOUNT

Login

Register

## Submissions & Workflow tasks

### Submissions

You may start a new submission.

The submission process includes describing the item and uploading the file(s) comprising it. Each community or collection may set its own submission policy.

### Archived Submissions

These are your completed submissions which have been accepted into DSpace.

Date accepted	Title	Collection
2016-08-01	Test.txt	Misc


### Workflow tasks

These tasks are items that are awaiting approval before they are added to the repository. There are two task queues, one for tasks which you have chosen to accept and another for tasks which have not been taken by anyone yet.

#### Tasks you own

Task	Item	Collection	Submitter
<input type="checkbox"/> Submission being reviewed	Testing Binary File 1	Misc	email: Kyriakos Ginis

[Return selected tasks to the pool](#)

#### BROWSE

[All of DSpace](#)[Communities & Collections](#)[By Issue Date](#)[Authors](#)[Titles](#)[Subjects](#)

#### MY ACCOUNT

[Logout](#)[Profile](#)[Submissions](#)

## Item submission

[Describe](#) [Describe](#) [Upload](#) [Review](#) [License](#) [Complete](#)

### Describe Item

#### Authors:

Last name, e.g. *Smith*

First name(s) + "Jr", e.g. *Donald Jr*

Add

Enter the names of the authors of this item.

#### Title: \*

Enter the main title of the item.

#### Other Titles:

Add

If the item has any alternative titles, please enter them here.

#### Date of Issue: \*

Year

Month

Day

Please give the date of previous publication or public distribution. You can leave out the day and/or month if they aren't applicable.