VI-SEEM project

Virtual Research Environment in Southeast Europe and the Eastern Mediterranean

https://vi-seem.eu

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The VI-SEEM project initiative is co-funded by the European Commission under the H2020 Research Infrastructures contract no. **675121**

Administrative details

- VRE for regional Interdisciplinary communities in Southeast Europe and the Eastern Mediterranean
- EINFRA-2014-2015; H2020

- Start date 01/10/2015
- Duration 36 months

- Total funded effort: 715 PMs
- EC contribution: 3.3 M euro

Geographical and historical context

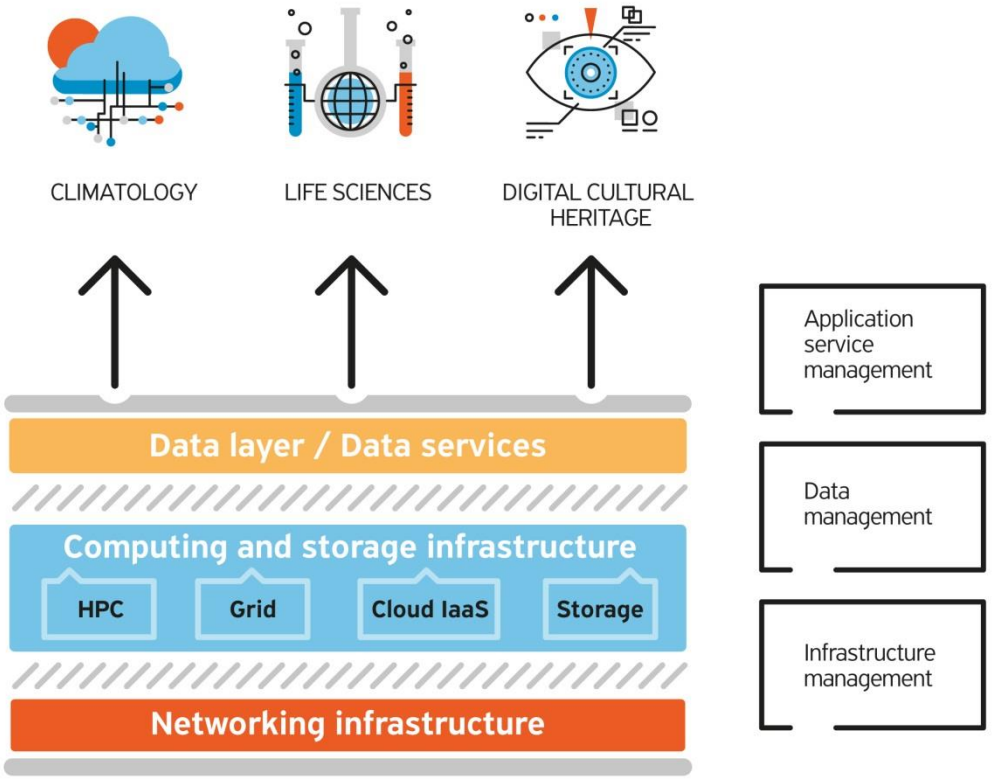
- VRE for regional Interdisciplinary communities in SEE and EM
- Merging of SEE and EM regions
- SEE: network SEEREN1-2, Grid SEE-GRID-1/2/SCI, HPC HP-SEE
- EM: HPC LinkSCEEM1-2

Participant no.	Participant organisation name	Part. short name	Country
1 (Coord)	GREEK RESEARCH AND TECHNOLOGY NETWORK S.A.	GRNET	Greece
2	THE CYPRUS INSTITUTE	CyI	Cyprus
3	INSTITUTE OF INFORMATION AND COMMUNICATION TECHNOLOGIES – BULGARIAN ACADEMY OF SCIENCES	IICT-BAS	Bulgaria
4	INSTITUTE OF PHYSICS BELGRADE	IPB	Serbia
5	NATIONAL INFORMATION INFRASTRUCTURE DEVELOPMENT INSTITUTE	NIIF	Hungary
6	WEST UNIVERSITY OF TIMISOARA	UVT	Romania
7	POLYTECHNIC UNIVERSITY OF TIRANA	UPT	Albania
8	UNIVERSITY OF BANJA LUKA	UNI BL	Bosnia and Herzegovina
9	SS CYRIL AND METHODIUS UNIVERSITY OF SKOPJE	UKIM	FYR of Macedonia
10	UNIVERSITY OF MONTENEGRO	UOM	Montenegro
11	RESEARCH AND EDUCATIONAL NETWORKING ASSOCIATION OF MOLDOVA	RENAM	Moldova
12	INSTITUTE FOR INFORMATICS AND AUTOMATION PROBLEMS OF THE NATIONAL ACADEMY OF SCIENCES OF THE REPUBLIC OF ARMENIA	IIAP-NAS-RA	Armenia
13	GEORGIAN RESEARCH AND EDUCATIONAL NETWORKING ASSOCIATION	GRENA	Georgia
14	BIBLIOTHECA ALEXANDRINA	BA	Egypt
15	INTER UNIVERSITY COMPUTATION CENTER	IUCC	Israel
16	SYNCHROTRON-LIGHT FOR EXPERIMENTAL SCIENCE AND APPLICATIONS IN THE MIDDLE EAST	SESAME	Jordan

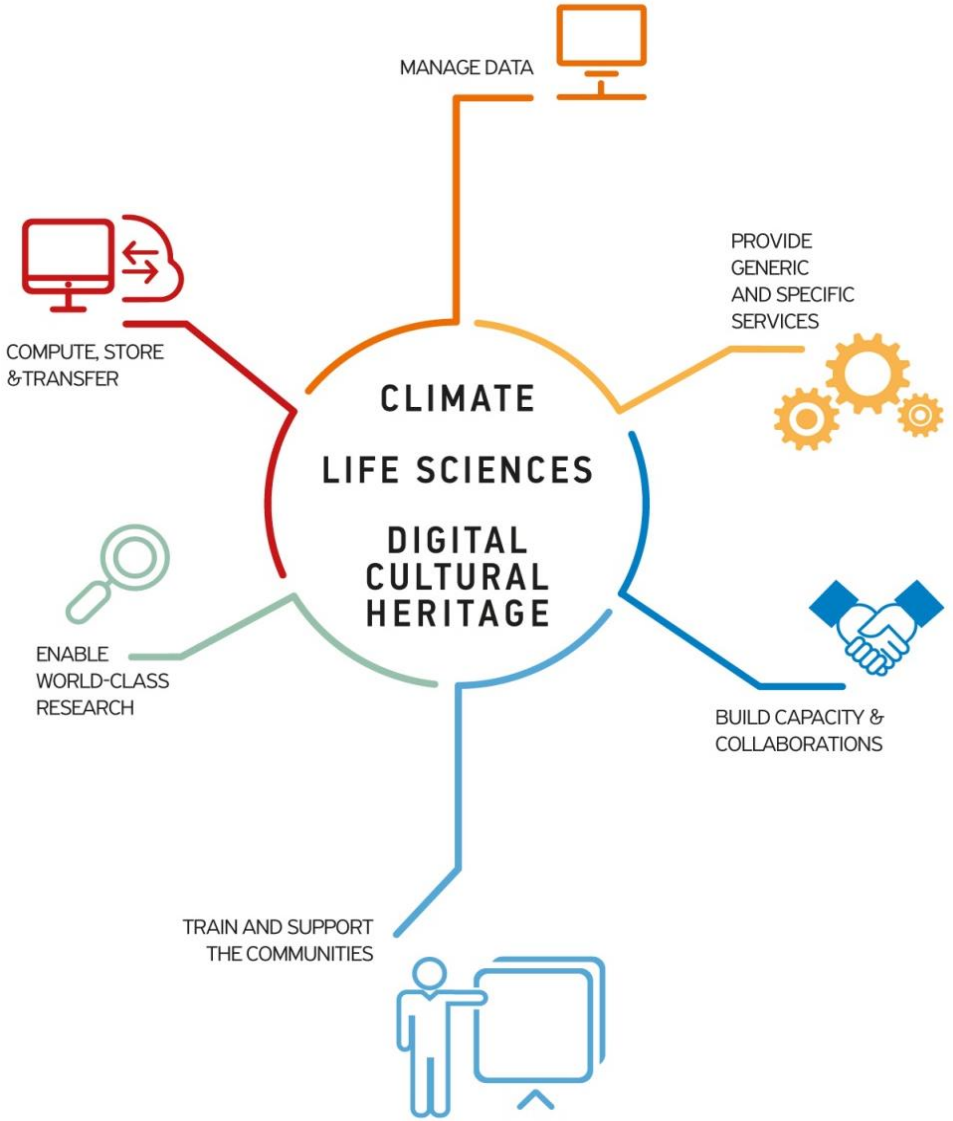
Technology context

- 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.

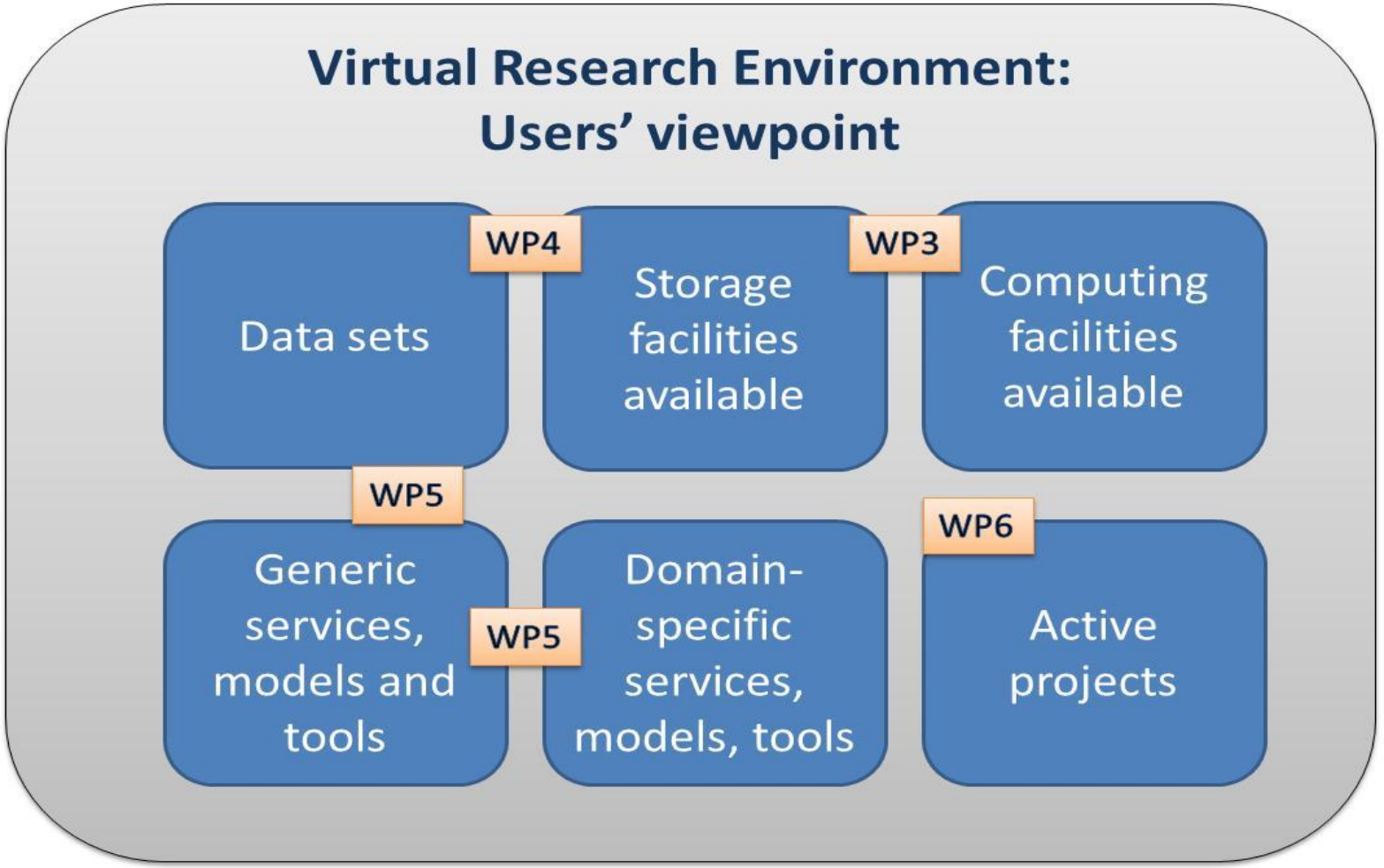
- Diverse computing technologies
- Advent of big data
- Service orientation



Detailed objectives



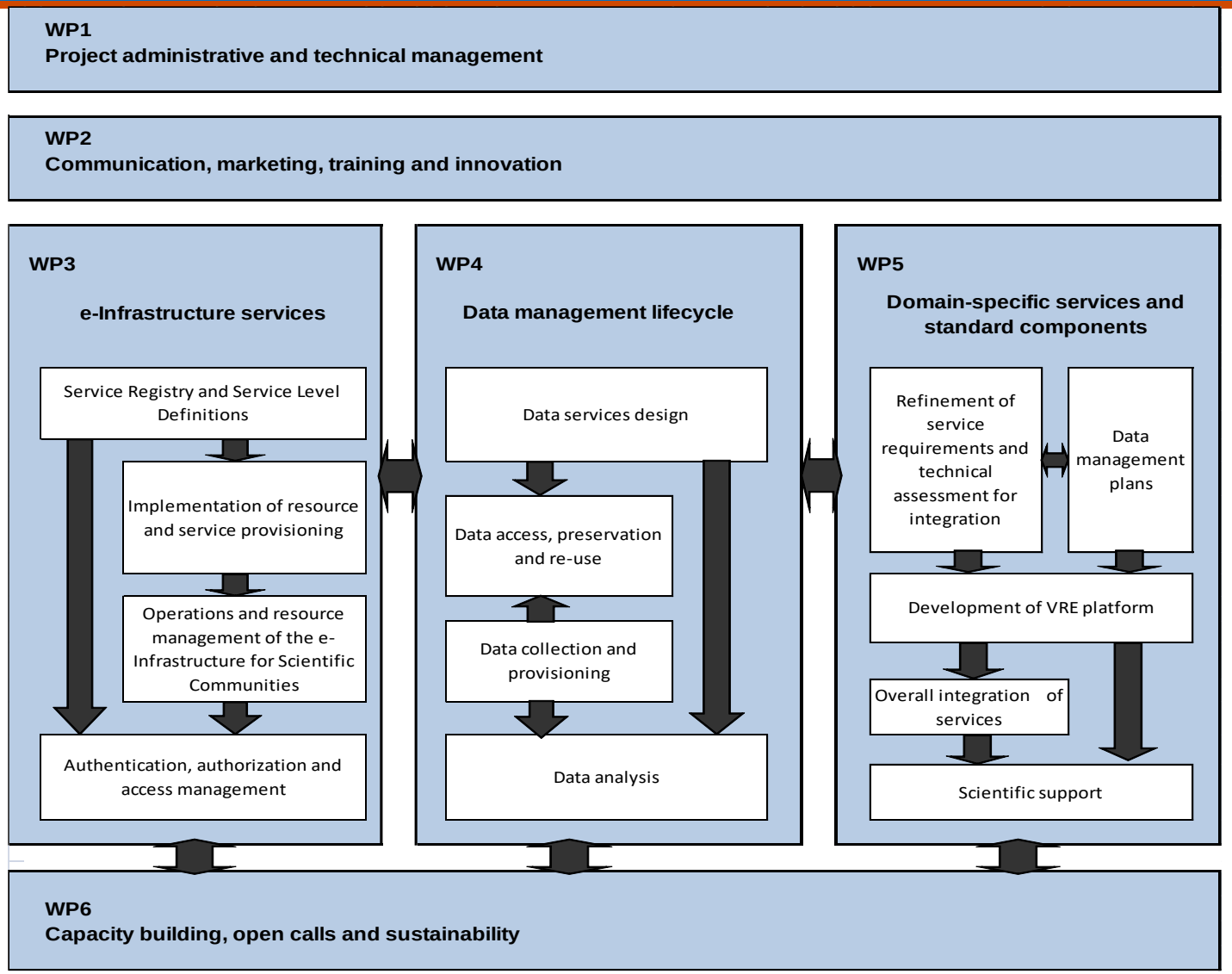
User-centric approach



Key Performance Indicators

- e-Infrastructure: **21500 CPU cores**, **325000** GP-GPU cores and 18500 Intel Xeon Phi cores of HPC, **2900 grid cores**, **10500 cloud VM cores**, **11 PBytes of storage** .
- > 10 specific services, 30 data sets and 25 codes
- 39 applications, 45 research teams taking part. 100 publications, 50 presentations
- 17 dissemination events,12 training events

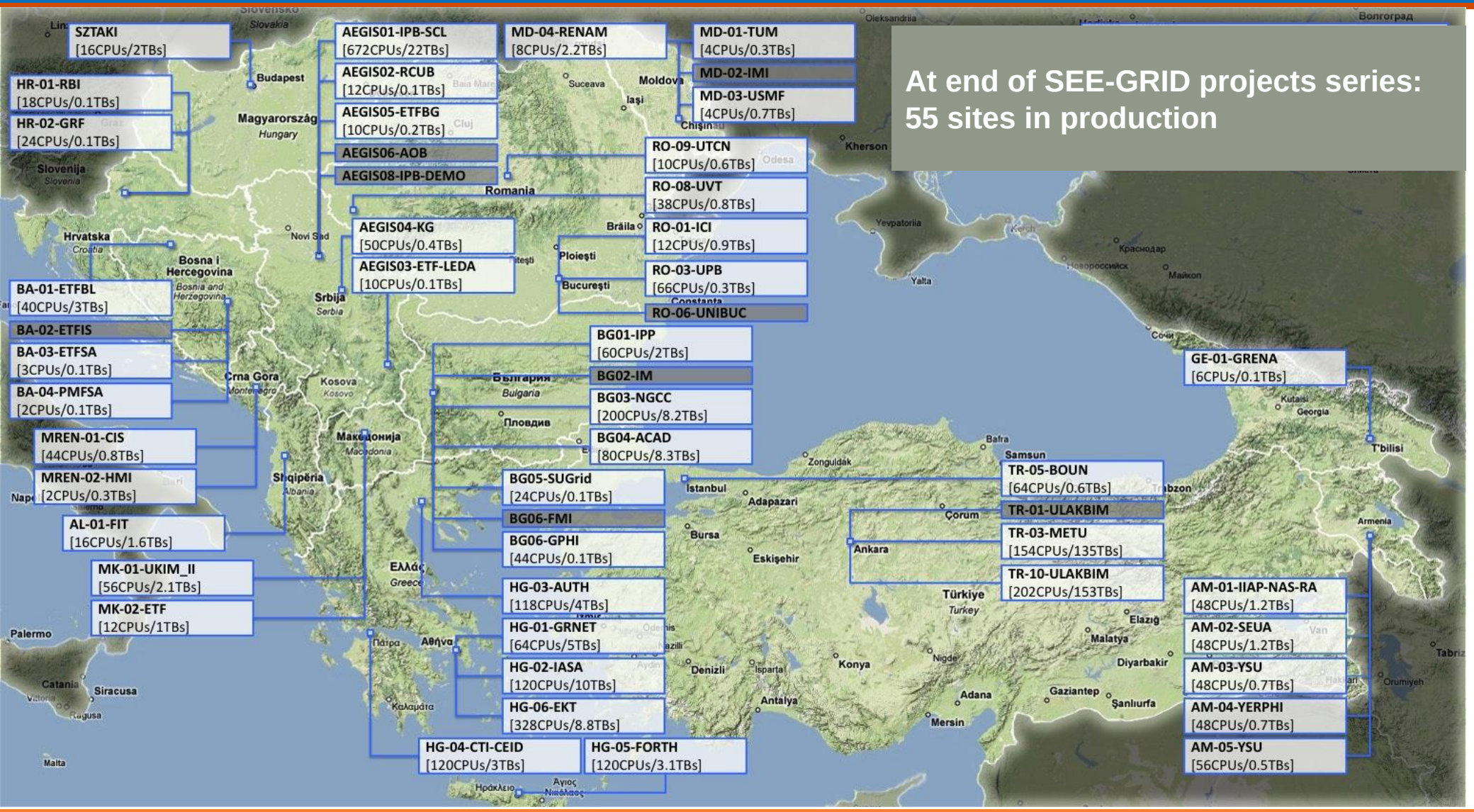
Work organisation



e-Infrastructures

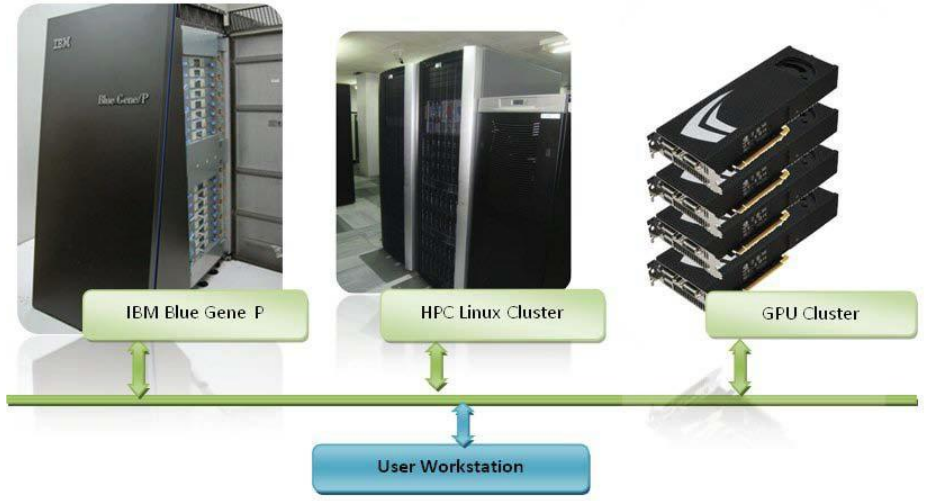
Resource Type	Number of countries contributing	Number of sites	Total amount of resources	Total amount of resources dedicated for the project
HPC x86 Compute	8	11	~21500 cores	~17.5 Million core hours per year
HPC GPU	3	3	~325000 GP-GPU cores	~ 18000 GPU cores
HPC Intel Phi Accelerators	1	1	~18500 co-processor cores	~8M co processor core hours per year
Grid Compute	12	25	~ 2900 cores	10-15% of the resources
Cloud Compute	8	9	~ 10500 VM cores	5% of VM cores
HPC Test/Train Cluster	3	4	~300 cores	~50000 cores hours per year
Storage (Disk)	13	18	3.1 PB	515 TB
Storage (Tape)	2	2	8 PB	550 TB

e-Infrastructures: Grid



e-Infrastructures: HPC

- 3 top 500 supercomputers in June 2015 (Bulgaria, Greece, Hungary)
- Heterogeneous infrastructure - Blue Gene/P SCs, large HPC clusters with advanced interconnects. Advantage to users
- To support a substantial number of libraries, toolkits, codes and application software



Data management

- Functions **allowing** for data management for selected Scientific Communities, engage the **full data management lifecycle**
- **Select and integrate data** management services tailored to the project's Scientific Communities
- **Deploy and operate** data management services that address the full data lifecycle
- **Collect the actual VRE-specific data sets** and make them available via common interfaces and services
- Data storage (live, dropbox-like), data archiving, data manipulation, collaborative access, domain specific interfaces to storage, data annotation and citation, metadata, PIDs, etc.

Types of applications

Climate	Life Sciences	Cultural Heritage
Regional Climate Modelling	**Modeling and Molecular Dynamics (MD) study of important drug targets**	Digital Libraries
Global Climate Modelling	Computer-aided drug design	Interactive Visualization Tools
Weather Forecasting	Analysis of Next Generation DNA sequencing data and RNA profiling data	Semantic Referencing
Air Pollution/Quality	Data mining to identify prevalent diseases/mutations in the SEEM region	Image Classification
Model Development	Image processing for biological applications	Modelling of Built Environments and Advanced Representation Techniques
Visualization, Datasets, etc.	Computational simulation of DNA and RNA	Scientific simulation of materiality and systems' properties
Other	Synchrotron data analysis	Geo-referencing Tools
	Other	Bioarchaeology

Access to VRE

- Through 3 distinct calls
- Pre-selected candidates project M12
- Open calls project M18 and M28 (1st closed)

University of Montenegro (UoM) contribution

- Parts of University of Montenegro in the project:
  - Department of electrical engineering
  - Department of natural sciences
  - Center of Information system
- Local team meetings to explore and define work plan
  - Application PSOMI (life science area): software used for research, data set preparations, technical support, analize of results, ..
  - Trainings

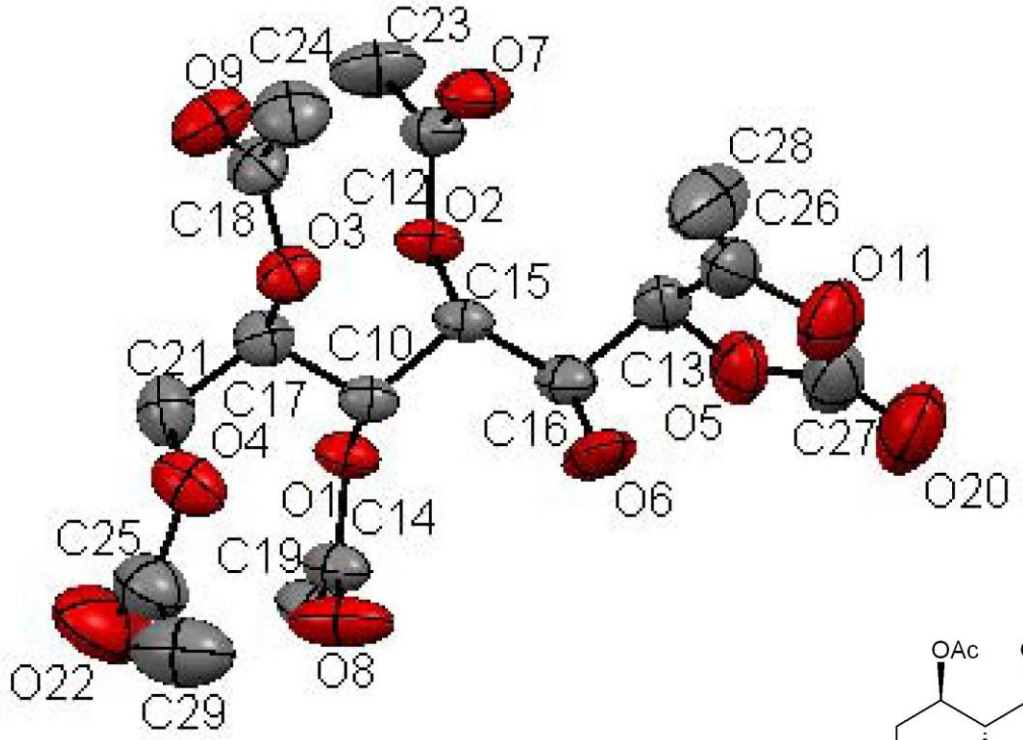
University of Montenegro (UoM) contribution

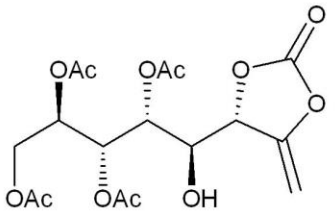
- Analysis of the storage requirements and user needs for the molecular dynamics research communities
- Data sharing and manipulation of produced results and used data
- Analysis of bank protein and selection of appropriate interaction
- **Preparing and creating dataset for molecules in 3D** (using applications Scatch Chem Chem Draw, namdb and Vega ZZ)
- **Creating dataset for the original molecule**, determination of the atoms arrangement and molecule topology file for (2R,3R,4R,5S)-5-hydroxy-5-((S)-methylene-2-oxo-1,3-dixolan-4-yl)-pentane-1,1,3,4-tetraacetate
- Simulations in GROMACS and NAMD.

PSOMI

- PSOMI simulations:
  - The selection of settings for the applications to create adequate interaction of the considered molecule with selected proteins using installed application
  - Determination of the optimal conformation of our selected molecule: (2R,3R,4R,5S)-5-hydroxy-5-((S)-methylene-2-oxo-1,3-dixolan-4-yl)-pentane-1,1,3,4-tetraacetate, with minimal repulsion of the atoms in space;
  - Examination the interaction between our molecule and the protein lysozyme, as a model interaction;
  - the examination of the interaction between our molecule and other membrane proteins (ongoing)
  - Interaction of our molecule with other proteins from RCSB database
  - Visualization of results (Vega ZZ)

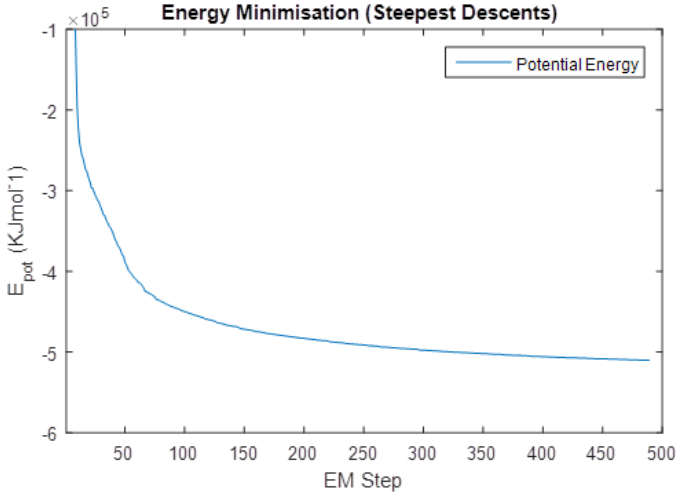
Data set for the molecule

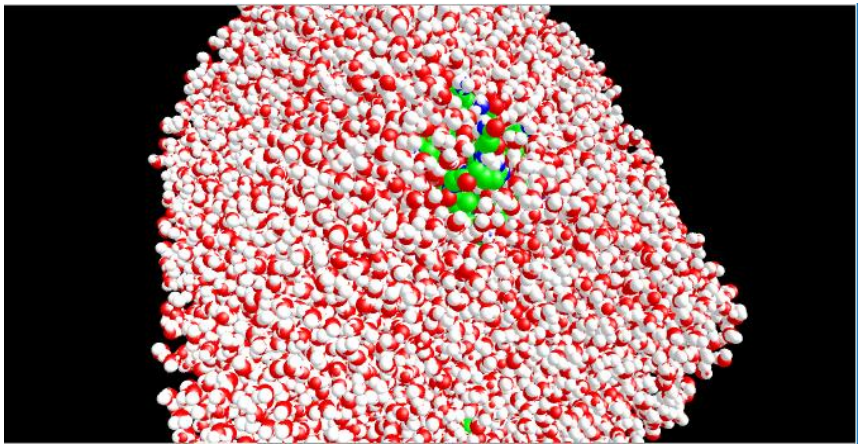


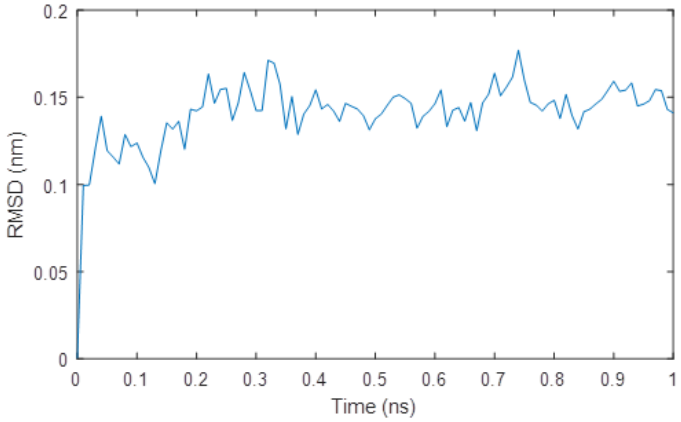


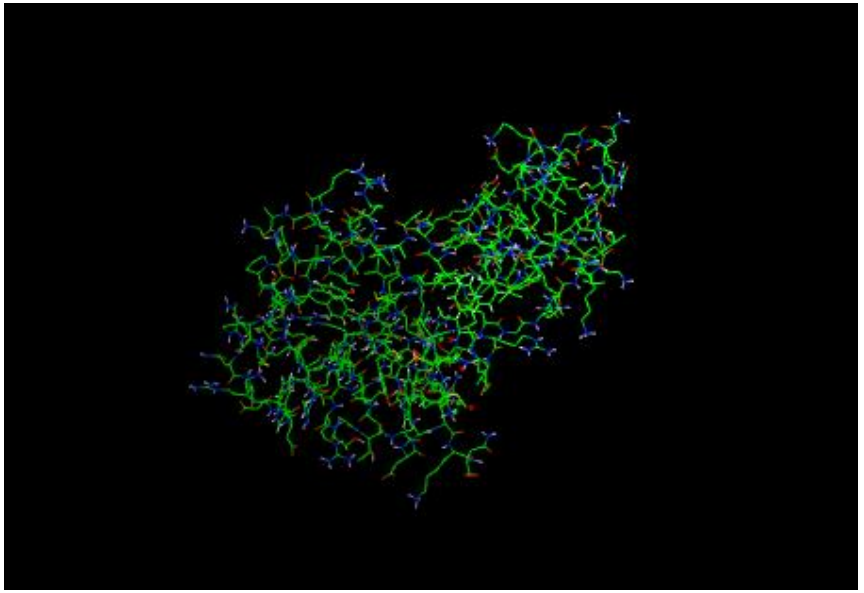
The considered molecule in 3D and its chemical structure

Simulation results (gromacs + vega ZZ)









University of Montenegro (UoM) plans

- Keep simulations interaction between molecule and cell membrane regarding identification of changes in structure of cell membrane
- Depending of obtained results, simulations with alternative molecule data sets
- Make some tutorial or training material regarding these simulatiions and share with VI SEEM services
- Comparive analisys of collected results in order to choose the best combination (the original molecule with proteins) for posible future implemetation (medicinal chemistry, drugs design, food production, etc.)
- Possible work on other applications (through open calls)

Conclusion

- SouthEast European initiatives built up the regional (and national) NRENs, NGI and HPC models
- LinkSCEEM project series linked the Eastern Mediterranean HPC facilities
- VI-SEEM unifies SEE and EM for the benefit of 3 large regional communities
- Virtual Research Environment to be provided to the scientific user communities in Climatology, Life Sciences, and Cultural Heritage
- VI-SEEM unifies networking, computing and data management
- Support in the full lifecycle of scientific research
- Services will be provided through a service catalogue

Thanks!

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