VRE User’s Manual
A Guide to the portals

Vi-SEEM
VRE FOR REGIONAL INTERDISCIPLINARY COMMUNITIES IN SOUTHEAST EUROPE & THE EASTERN MEDITERRANEAN
Explore > Exploit > Excel
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1. The VI-SEEM Virtual Research Environment

1.1. 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 (SEEM).

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.

You can visit VI SEEM website at https://vi-seem.eu/.

1.2. How do you access the VI-SEEM Virtual Research Environment?

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

1.3. VI-SEEM Services

The VI-SEEM 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. All the services can be found at the VI-SEEM Service Catalogue & portfolio which can be found at https://services.vi-seem.eu. VI-SEEM Service Catalogue/portfolio is described in Section 1.7.

VI-SEEM provides the following services:
1.3.1. **VI-SEEM scientific application environment**

This service provides access and information to several modules such as optimized applications and libraries, Virtual Machine (VM) images and list of codes, relevant to the work of the regional scientific communities of interest. The Scientific application environment can be accessed through the header of the VRE-portal [https://vre.vi-seem.eu/](https://vre.vi-seem.eu/).

1.3.2. **Workflow and software tools repository**

This service provides access and information to 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. The Workflow and software tools repository can be accessed through the header of the VRE-portal [https://vre.vi-seem.eu/](https://vre.vi-seem.eu/).

1.3.3. **Regional community datasets**

This service provides access and information regarding datasets of regional importance for the scientific communities of interest. The Regional Community datasets are organized according to the Scientific Disciplines:

- **Climate**
  - Weather Datasets
  - Analysis Datasets
  - Air Quality Datasets
  - Regional Climate Datasets

- **Life Sciences**
  - Modeling and Molecular Dynamics Datasets
  - Computer aided Drug Design Datasets
  - Analysis of Next Generation Sequencing Datasets
  - Synchrotron Data Analysis Datasets
  - Image Processing For Biological Applications Datasets
  - Computational Simulation of DNA and RNA Datasets

- **Digital Cultural Heritage**
  - Digital Libraries
  - Machine Learning for Digital Cultural Heritage
  - Online Visualization Tools

The Regional community repository can be accessed through the header of the VRE-portal [https://vre.vi-seem.eu/](https://vre.vi-seem.eu/).
1.3.4 Application-level services

This category provides Web-based or visualization services enabling easy access to underlying workflows, applications, and resources. The Application-level services can be accessed through the header of the VRE-portal. Currently there are seven available Application-Level Services:

1.3.4.1 Application-level services in Climate Research

**Live Access Server** ([http://las.vi-seem.eu](http://las.vi-seem.eu))

Live access server is a highly configurable server designed to provide flexible access to georeferenced 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.

1.3.4.2 Application-level services in Life Sciences Research

- **Subtract** ([http://subtract.vi-seem.eu/](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.

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/](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 preexisting 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/](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](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.

1.3.4.3  **Application-level services in Digital Cultural Heritage**


  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.
1.4 VI-SEEM VRE portal


**Description:** The Virtual Research Environment Portal is the portal which connects the user to the VI-SEEM services. It has a user-friendly structure and can easily direct the user according to the desired result. The portal connects the unified infrastructure, the generic services and hosts the user-tailored front end interface. This integrated platform enables easy communication and data sharing between the various user groups. The navigation of the user can be done through the header of the front page or the layout.

1.4.1 Header

The header of the VRE-portal provides the following tabs

1. **Scientific Application Environment**

   The Scientific application environment services provides the list of Service Enablers, also contains links to the climate, cultural heritage, and life science Applications and Libraries, Virtual Machine (VM) images and Software developed use cases. Furthermore it provides guidelines on HOW TO CONTRIBUTE to Scientific Application Environment.

2. **Workflows, Software Tools**

   Workflow and software tools repository provides several modules such as documents containing best practice procedures and workflows for the production of results relevant to the application categories identified in the SEEM region. Here you can find links to pages containing lists with short description and access/documentation details for the scientific workflows provided by the VI-SEEM platform, and list of the codes that can currently be download from the code repository arranged by scientific community. Furthermore it provides guidelines on HOW TO CONTRIBUTE to Workflows and Software tools.
3. **Regional Community Datasets**

Regional community datasets tab provides scientific data, publications and simplified data formats for immediate re-use organized into **Climate Scientific Community Datasets**, **Digital Cultural Heritage Scientific Community Datasets**, and **Life Sciences Scientific Community Datasets** followed with instructions HOW TO CONTRIBUTE to datasets.

4. **Application-level Services**

Application-Level Services tab provides links to the associated application-level services of the three scientific communities as well as instructions on HOW TO CONTRIBUTE TO THE APPLICATION LEVEL SERVICES.

### 1.4.2 Layout of the VRE-portal

The layout of the VRE-portal has been designed so that could provide the user the needed information and material in an easy way. This is manifested through the organization of the page in the following sections:

1. **User Zone**: this provides access according to the user orientation/experience/needs.
2. **VI-SEEM support the following Scientific Communities**: it is organized in disciplines.
3. **Cross Disciplinary Fields**: This section exploits the cross-disciplinarity character of the provided material.
4. **VI-SEEM Sites**: Provides access to the main VI-SEEM websites
5. **European Infrastructure Projects**

#### 1.4.2.1 User Zone

This section provides tabs for linking users to the right places:
• **Researchers**: From these parts of the webpage a Researcher could be linked to directions on how to:
  - Apply for Computational Resources
  - Access the Source Code Repository
  - Access to the supported applications & libraries
  - Access the Scientific Workflows
  - Access the Datasets
  - Access the Application-level Services
  - Access the VI-SEEM training portal

• **Students**: From this part of the webpage a student could find directions on how to:
  - Access the VI-SEEM Training Portal
  - Access the Events Calendar
  - Access the Source Code Repository
  - Access to the supported applications & libraries
  - Access the Scientific Workflows
  - Access the Datasets

• **SMEs**: This section of the webpage is dedicated for SMEs, and provides all the necessary information to:
  - Apply for Computational Resources
  - Access the Datasets
  - Access the Use Cases

• **Regional Resources Available**: This section provides access to information related to the available:
  - VI-SEEM Compute Resources
  - VI-SEEM Data Resources

• **VI-SEEM Service Catalogue & Portfolio**: This section provides access to the Service Catalogue & Portfolio.

• **Use Cases**: This section directs the reader to use cases developed throughout the VI-SEEM Integration phases as well as the Open Calls. The two links take the visitor to:
  - Explore VI-SEEM Datasets
  - Developed Use Cases
1.4.2.2 **VI-SEEM VI Support the following scientific Communities**

This section of the VRE-portal is organized according to the Scientific Discipline of the visitor. Namely, it is configured in three silos one for each community (Climate, Life Sciences, Digital Cultural Heritage) each one containing links on related material on the following:

- **Application-Level Services**
- **Datasets**
- **Codes**
- **Workflows**
- **Optimized Applications and Libraries**

![VI-SEEM support the following Scientific Communities](image)

1.4.2.3 **Cross Disciplinary Fields**

This section reflects to the Cross-Disciplinary character of VI-SEEM. Thus, instead of the Scientific Discipline (Silo) orientation of an application or a datasets etc. this section provides a horizontal categorization according to the type of material which can be used in more than one discipline. The structure of this section as this is illustrated in the next picture:

![Cross Disciplinary Fields](image)

By clicking on one of the following 5 subsections:

- Data Visualization
- Simulation Data
- Data Analytics and Processing
- Analytical Studies & Portfolio
- Source Code

the user is directed in a webpage which is graphically organized by the following Venn diagram
By clicking on one of the discipline-overlapping areas the user is directed to the right section of the webpage.

By clicking on the subsection

- Geographic Datasets

The user is directed a webpage which is graphically organized by the following SEEM map:

By clicking on a VI-SEEM Partner country the user is directed to a list with projects associated with Geographic Datasets of the given country. Such projects may involve Georeferencing, Remote Sensing, etc.

1.4.2.4 **VI-SEEM Sites**

This section provides links to the VI-SEEM website, to the VI-SEEM Training Portal, to the VI-SEEM Code Repository as well as to the VI-SEEM Wiki.
1.4.2.5 European Infrastructure Projects

This section provides links to other Infrastructure projects which might be of the interest of the user. This section lists projects such as PRACES, EGI, EUDAT, GEANT and OpenAIRE as well as projects with a DCH orientation such as ARIADNE, CLARIN, DARIAH, E-RHIS and GRAVITATE:

Finally the VRE-Portal optionally asks the user to provide feedback. So please dedicate a couple of minutes to provide, valuable to us, information and comments about the portal.

1.5 VI-SEEM training portal

Access the VI-SEEM training portal: http://training.vi-seem.eu/.

Description: The VI-SEEM training portal collects and curates training material for the VI-SEEM services. Through the use of the training portal users have access to information for the available e-infrastructure services (HPC, Grid, Cloud and Data) as well domain specific material for using the tools and data provided. The VI-SEEM training portal is the main source of the training material for the VI-SEEM users and it offers a number of important features which make the portal user friendly. The training-portal has an enhanced user oriented character, which provides easy access to researchers, students and users in general.

Content:
The front page of the training portal consists of a header which provides access to the following training Material:

- Domain Specific Software and Tools
- Data and Visualization
- Common Computing Resources
- Event Related Training Material

In addition the header of the training portal provides a search engine.
The front page of the training portal, shown in Figure 1, has a high-level organization structured in three main categories:
• **Domain Specific Software and Tools** providing access to training material for
  - Climate Software and Tools
  - Digital Cultural Heritage Software and tools
  - Life Science Software and Tools

• **Data and Visualization** providing access to training material for:
  - Data
  - Storage Services
  - Visualization

• **Common Computing Resources** providing access to training material for
  - Cloud
  - High Performance Computers
  - Grid

Therefore, the training portal is organized in nine sections each one described by a distinct icon. By clicking on the icon the user is directed to the associated training material. In the next subsections we provide a description on the structure of each one of the nine sections.

![Figure 1. The front page of the Training Portal](image-url)
1.5.1 Climate Software and Tools

From this webpage the user can access all the training material which is related to the VI-SEEM Climate applications as well as training material which is related to general software applications, modules and data structures used by the Climate Scientific Community. The structure of the webpage follows the needs of the Climate researchers within the VI-SEEM Project. Hence, the layout of the webpage is organized in five sections (tabs):

- Live Access Server
- VI-SEEM Applications
- Visualization
- Software and tools
- General Training Material

The first tab provides access to the training material on the Live Access Server. The second tab provides access to training material on the Climate applications which have been integrated in the VRE during the three integration phases. The associated training material is organized in three sections. These sections are chosen to reflect the Climate Research areas supported by VI-SEEM:

- Regional Climate Modelling
- Air Quality
- Weather Forecast

An important tool which enables Climate Scientists demonstrating their results effectively is Visualization applications for climate. Therefore, the third tab is dedicated on Visualization. The next tab focusses in Software and tools; namely it provides training material on the WRF and RegCM software as well as on NetCDF data format. Finally, more general training material is provided in the last tab.

1.5.2 Digital Cultural Heritage Software and tools

From this webpage a user interested in VI-SEEM Digital Cultural Heritage applications can find the corresponding training material. The structure of the page has been designed in such a way so that it enhances its efficiency and reduces the time a user needs to seek for training material. Since the Digital Cultural Heritage community has a strong application-driven character, the webpage is organized in the following seven tabs named after the particular application and action:

- Clowder
- Vi-SEEM applications
- Content Management Systems
- Metadata
- Digitization
- Visualization
- General Training Material

The first tab provides access to training material on the Clowder.

Subsequently VI-SEEM provides access to the training material related to the VI-SEEM applications developed in the three integration phases. The corresponding training material is organized in the following three sections:
The Remaining five tabs provide access to training material related to Content Management Systems, Metadata, Digitization, Visualization and General Training Material.

### 1.5.3 Life Science Software and Tools

A user can find all the training material related to the Life Sciences applications supported by VI-SEEM. The structure of this page has been tailored to the needs of the Life Scientific Community. It is organized in four tabs named after the corresponding research area:

**Molecular Dynamics Simulations**
- Molecular Dynamics Simulations
- Computer Aided Drug Design
- Next Generation Sequencing Data Analysis
- Medical Image Processing

Each one of these tabs is subsequently organized in three distinct sections:
- **General Training Material**: This involves training material related to the application modules used in the particular research area.
- **VI-SEEM applications**: This includes training material related to the developed VI-SEEM Life applications.
- **Application Level Services**: This consists of the material, mostly tutorials, on how a user can use the particular Application-Level Service. For instance, there the user can find tutorials and presentations on the usage of ChemBioServer, AFMM, Nano-Crystal, Subtract and DICOM Network.

### 1.5.4 Data

Data related training material can be accessed in this section. The structure of this page has been tailored according to the relation of the Scientific Communities with their data consideration. It is organized in three tabs:

- **General Training Material**
- **Climate**
- **Digital Cultural Heritage**

### 1.5.5 Storage Service

Training Material related to Storage Services is available in this section. We provide training material dedicated to the VI-SEEM Data Repository as well as to VI-SEEM Simple Storage Service.

### 1.5.6 Scientific Visualisation

This page provides material for training purposes on Scientific Visualization. This page is organized in three sections-tabs. This structure is in accordance with the cross-disciplinary character of VI-SEEM, thus we provide General Training Material which can be used by all three
Scientific Communities. In addition we include Visualization Topics focusing on the scientific communities of Climate and Cultural Heritage. Thus, the tabs appearing in the webpage are the following:

- General Training Material
- Climate
- Digital Cultural Heritage

### 1.5.7 Cloud

Training Material focusing on Cloud computing can be obtained from this webpage. The page is self-contained and is not organized in tabs.

### 1.5.8 HPC

Training material on High Performance Computers (HPCs) can be accessed through this page. This webpage provides the user with four options manifested by four distinct buttons:

- Practical HPC
- Development
- Improvement
- Applications

“Practical HPC” provides all the documentation and training needed to access and run a supercomputer. This part of HPC training consists of four different sections/tabs:

- Super Computer Basics
- Scripting
- Version Control
- Parallel Tools Platform

“Development” provides all the information one needs to know in order to develop an application capable to run on computers making use of multi-core architectures. The training material on Development is provided in six tabs:

- Programming
- Python
- OpenMP
- MPI
- GPU Programming
- General Training Material

“Improvement” provides documentation on topics which enable the user to analyze the performance of codes as well as to improve the codes and debug them. Optimizing a code running on HPCs is an important task which reduces the execution time and makes the runs less expensive in terms of power consumption. This part of the HPCs’ training material splits in two tabs:
Finally “Applications” provide a number of cross-disciplinary documentations focusing on particular applications which make use of HPCs. Such applications are Synchrotron software and imaging software running on multicore architectures.

### 1.5.9 GRID

Training material focusing on GRID computing can be accessed in this section. The page provides sliders with links to training material on several aspects of Grid computing.
1.6 VI-SEEM wiki


**Description:** The VI-SEEM wiki aims to support site managers for operating the integrated VRE services on top of the underlying infrastructures. It contains information about the available services, the procedures for integrating existing services with the VI-SEEM e-infrastructure and how-to material for establishing new services and integrating them with the existing VRE services.

**Contents:**

1. Infrastructure Resources
   - HPC Resources
   - Cloud Resources
   - Grid Resources
   - Storage Resources

2. Access to Resources
   - VI-SEEM Login
   - VI-SEEM Login Integration Guide
   - Access to VI-SEEM e-Infrastructure Resources

3. VI-SEEM Service Catalog/Portfolio

4. Operations and Resource Management
   - GOCDB
   - Monitoring
   - Accounting
   - Helpdesk

5. Source Code Repository

6. Data Services
   - iRODS Documentation

7. Service and Application Enabling

8. Training

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**Figure 2:** The content of the front page of VI-SEEM wiki
1.7. VI-SEEM service catalogue/portfolio

Access VI-SEEM service catalogue/portfolio:
https://services.vi-seem.eu/ui/catalogue/services/

Description: This portal VI-SEEM offers a broad set of generic as well as application specific services. Such services are in the areas of Compute resource provisioning (HPC, Grid and Cloud), Storage and Data services provisioning, Data Set provisioning, Software and Scientific Workflow provisioning as well as Application Specific service provisioning. These services creating a unique Virtual Research Environment (VRE), thus improving research productivity and competitiveness on the pan-European level.

Content:

- Data Storage
  - VI-SEEM Data Discovery Service
  - VI-SEEM Archival Service
  - VI-SEEM Simple Storage
  - VI-SEEM Repository

- Application Specific
  - Subtract
  - ChemBioServer
  - VI-SEEM Regional Community Datasets
  - VI-SEEM Live Access Server
  - AFMM
  - VI-SEEM Scientific Application Environment
  - VI-SEEM Workflow, software tools repository
  - NANO-Crystal
  - DICOM
  - VI-SEEM Clowder

- Compute
  - VI-SEEM Cloud
  - VI-SEEM HPC
  - VI-SEEM Grid

- Authentication and Authorisation
  - VI-SEEM Login

- Service provisioning
  - VI-SEEM Service Portfolio Management System
VI-SEEM Service Catalogue

VI-SEEM offers a broad set of generic as well as application specific services in the region of Southeastern Europe and Eastern Mediterranean, with special focus on the scientific communities of Life Sciences, Chronology and Digital Cultural Heritage. Such services are in the areas of Compute resource provisioning (HPC, Grid and Cloud), Storage and Data services provisioning, Data set provisioning, Software and Scientific Workflow provisioning as well as Application Specific service provisioning. These services create a unique Virtual Research Environment (VRE), thus improving research productivity and competitiveness on the pan-European level.

- Data Storage
  - VI-SEEM Data Discovery Service
  - VI-SEEM Archival Service
  - VI-SEEM Simple Storage
  - VI-SEEM Repository

- Application Specific
  - Subtract
  - ChemBioServer
  - VI-SEEM Regional Community Datasets
  - VI-SEEM Live Access Server
  - AFMM
  - VI-SEEM Scientific Application Environment
  - VI-SEEM Workflow, software tools repository
  - NANO-Crystal
  - DICOM
  - VI-SEEM Clowder

- Compute
  - VI-SEEM Cloud
  - VI-SEEM HPC
  - VI-SEEM Grid

- Authentication and Authorisation
  - VI-SEEM Login

- Service provisioning
  - VI-SEEM Service Portfolio Management System

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**Figure 3.** The content of the Service Catalogue as this is presented in the [https://services.vi-seem.eu](https://services.vi-seem.eu) webpage.
1.7 Code repository

Access the Code Repository: https://code.vi-seem.eu/

**Description:** VI-SEEM Code repository hosts tools, software and workflows made available from the VI-SEEM Scientific Application environment. It is deployed on top of the git open source system. GitLab is used to provide a usable web-based UI for project management and repository control. The service is fully integrated with VI-SEEM Login service.

![Image of the code repository front page](image)

*Figure 1: The front page of the code repository*
1.8 VI-SEEM repository

Access the VI-SEEM repository: https://repo.vi-seem.eu/

**Description:** The VI-SEEM Repository provides long-term data preservation, suitable for data set sharing. VI-SEEM repository is based on DSpace. DSpace is an open source repository software package typically used for creating open access repositories for scholarly and/or published digital content. DSpace shares some features with content management systems and document management systems. In addition the DSpace repository software serves a specific need as a digital archives system, focused on the long-term storage, access and preservation of digital content.

The repository can be used for a variety of use cases like:
- Storage of curated datasets for longer term preservation
- Sharing those datasets with selected collaborators or opening them up to entire communities, via a web interface
- Making such data sets searchable by means of associating metadata and then harvesting them
- Enabling scientific communities to capture and describe digital works using a custom submission workflow module. The VI-SEEM Repository is available at https://repo.vi-seem.eu/

**Content:**
- Communities in DSpace
  - VI-SEEM Climate Sciences
  - VI-SEEM Digital Cultural Heritage
  - VI-SEEM Life Sciences
  - Vi-SEEM Project Community
- Recently Added

![Figure 4 The VI-SEEM Repository front page](image-url)
1.9 Support ticket system

Access the Support ticket system: https://support.vi-seem.eu/

Description: The support ticket system represents an osTicket installation hosted at the University of Banja Luka. Agent login is located at https://support.vi-seem.eu/skp and is to be used by support personnel of the project. Help topics currently include generic topics (feedback and reporting a problem) as well as VI-SEEM specific topic including: Infrastructure, Service Registry, Data Platform, Applications and Domain Specific Services.

Content:
1. Open a New Ticket
2. Open Ticket Status

![Image of the support ticket system front page]

Figure 5 The front page of the support ticket system
1.8. Available Workflows

In the following three sections we provide a list of the available workflows in the VRE-Portal for each scientific discipline respectively. All the titles are clickable and direct the user to the workflow.

1.8.1. Climate

1.8.1.1 VINE: Setup and run WRF-Chem model over the south Caucasus domain

**Description:** Vine provides improved research in process-level understanding considering to the coupling and feedbacks above the territory of Georgia: dust emission; dust ageing; dust deposition.

1.8.1.2 VisTrails Training Workflow

**Description:** VisTrails is an open-source scientific workflow and provenance management system that provides support for simulations, data exploration and visualization. Whereas workflows have been traditionally used to automate repetitive tasks, for applications that are exploratory in nature, such as simulations, data analysis and visualization, very little is repeated—change is the norm. As an engineer or scientist generates and evaluates hypotheses about data under study, a series of different, albeit related, workflows are created while a workflow is adjusted in an interactive process. VisTrails was designed to manage these rapidly-evolving workflow.

1.8.1.3 WRF Installation Workflow & WRF Check Output and Troubleshooting workflow

**Description:** WRF is a next-generation mesoscale numerical weather prediction system designed for both atmospheric research and operational forecasting applications. It features two dynamical cores, a data assimilation system, and a software architecture supporting parallel computation and system extensibility. The model serves a wide range of meteorological applications across scales from tens of meters to thousands of kilometers. The effort to develop WRF began in the latter part of the 1990's and was a collaborative partnership of the National Center for Atmospheric Research (NCAR), the National Oceanic and Atmospheric Administration (represented by the National Centers for Environmental Prediction (NCEP) and the (then) Forecast Systems Laboratory (FSL)), the (then) Air Force Weather Agency (AFWA), the Naval Research Laboratory, the University of Oklahoma, and the Federal Aviation Administration (FAA).

1.8.1.4 TVRegCM Workflow

**Description:** Tuning and Validation of the RegCM – Adaptation and tuning of the RegCM model for the Balkan Peninsula and Bulgaria and thus development of a methodology able to predict possible changes of the regional climate for different global climate change scenarios and their impact on spatial/temporal distribution of precipitation, hence the global water budgets, to
changes of the characteristics and spatial/temporal distribution of extreme, unfavorable and catastrophic events (drought, storms, hail, floods, fires, sea waves, soil erosion, etc.). All these changes will have influence on the ecosystems and on practically all sectors of the economy and human activity and consequently on the quality of life.

1.8.1.5 **ACIQ Workflow**

**Description:** Atmospheric Composition Impact on Quality of Life and Human Health – Development of a methodology and performing reliable, comprehensive and detailed studies of the impact of lower atmosphere parameters and characteristics on the quality of life (QL) and health risks (HR) for the population in our country.

1.8.1.6 **ClimStudyArmenia Workflow**

**Description:** Accurate Prediction and Investigation of Weather and Climate in Armenia and South Caucasus – Methods and methodologies for accurate weather prediction and climate change based on series of experiments, as mountainous terrain of the country, the apparent ruggedness of the terrain, the big difference between relative altitudes, as well as atmospheric general circulation features make it challenge. This is a WRF application.

1.8.1.7 **Calculation of Anharmonic X-H Stretching Frequencies of Intramolecular Vibrational Chromophores Relevant to Atmospheric Chemistry**

**Description:** Calculation of Anharmonic X-H Stretching Frequencies of Intramolecular Vibrational Chromophores Relevant to Atmospheric Chemistry – In the present scientific workflow, through the example of this simplest organic acid an illustration of the approach to compute the anharmonic vibrational frequencies of characteristic X-H intramolecular chromophores which are treatable within 1D approximation (i.e. as one-dimensional anharmonic oscillators) will be shown. The approach is straightforwardly extendable to an arbitrary X-Y oscillator.

1.8.2. **Life Sciences**

1.8.2.1 **Membrane protein tutorial with GROMACS**

**Description:** This tutorial describes a series of steps to set up and run an MD simulation of a membrane protein embedded in a solvated lipid bilayer using the GROMACS program and its associated tools.

1.8.2.2 **Molecular Dynamics Simulations of BPTI in Vacuum**

**Description:** The main objective of this practical is to provide an overview of classical Molecular Dynamics (MD) simulations and Normal Mode Analysis (NMA) by examining the protein called bovine pancreatic trypsin inhibitor (BPTI) within the framework of the CHARMM program.
1.8.2.3 **Molecular Dynamics simulations of lysozyme in water**

**Description:** The main objective of this practical is to provide an overview of classical Molecular Dynamics (MD) simulations and Normal Mode Analysis (NMA) by examining the protein Lysozyme within the framework of the NAMD program.

1.8.2.4 **PSOMI Workflow**

**Description:** This workflow contains steps for analysis interaction between small ligand and protein by using ChemSketch, Open Babel, PRODRG and Gromacs on HPC cluster. Workflow uses complex of small ligand and protein as input file (in .gro format), and gives trajectories (.trr extension) that further can be analysed in VMD or similar software.

1.8.2.5 **Usage of CCC Code**

**Description:** This workflow provides all the information needed for running the Classification of cancer cells application. The purpose of this application is the development of an advanced approach for X-ray images in the context of signal processing, enabling medical users to diagnose automatically cancer cells.

1.8.2.6 **THERMOGENOME Workflow**

**Description:** Workflow for measurement of thermodynamic stability of RNA/DNA and DNA/DNA duplexes. Perl software scripts for measurement of thermodynamic stability of RNA/DNA and DNA/DNA duplexes.

**Accompanying codes/scripts:** THERMOGENOME Perl script

1.8.2.7 **CNCADD Workflow**

**Description:** CNCADD application provides a comparison of conventional with novel models for computer assisted drug delivery simulation, using methodologies including molecular dynamics, statistical physics, and Monte Carlo.

**Accompanying codes/scripts:** CNCADD Fortran Code

1.8.2.8 **Best Practices for NGS1**

**Description:** NGS1 application provides application of NGS technology and pipeline to address the identification of genetic mutations that cause rare diseases in families and of genetic variants that contribute to complex diseases such as autism and cancer.
1.8.2.9 **Best Practices for NGS2**

**Description:** This document is written as a guide with examples on how to perform alignment of NGS data and avoid various pitfalls.

1.8.2.10 **Calculation of Local Mode Frequencies (Partial Vibrational Density of States) from Classical or AB Initio Molecular Dynamics Simulations**

**Description:** Calculation of Local Mode Frequencies (Partial Vibrational Density of States) from Classical or AB Initio Molecular Dynamics Simulations – In this scientific workflow a method for efficient processing of the results from MD simulations is presented. In the particular case considered, the results from Born-Oppenheimer MD (BOMD) simulations, generated either with Gaussian09 or ORCA 4.0 series of codes will be used.

1.8.2.11 **Mol_Surf Workflow**

**Description:** Mol_Surf – Recommended workflow for equilibrium molecular dynamics simulations with Gromacs 5.1 of surfactants adsorbed at the vacuum/water interface as well as the accompanied scripts/files.

**Accompanying Scripts:** prod.mdp, queue_script.pbs, heat.mdp, min.mdp, relax.mdp, surfactants_water.top

1.8.2.12 **MULTIDRUG Workflow & MULTIDRUG Workflow Chart**

**Description:** MULTIDRUG – Recommended workflow description for atomistic molecular dynamics simulation of biomolecules with GROMACS 5.1.

**Accompanying Scripts:** heat.mdp, membrane.top, min_env.mdp, min_whole.mdp, prod.mdp, relax.mdp, run_mdrun.pbs

1.8.3. **Digital Cultural Heritage**

1.8.3.1 **Manuscript workflow**

**Description:** Manuscript application provides a tool for automatic processing of historical documents, enabling scholars to access and process historical documents efficiently. The workflow is an article explaining how the Manuscript code works.
1.8.3.2 VirMuf Pipeline

**Description:** VirMuf application provides a tool that complements and enriches the real museum, substitutes for the inability to visit it, adds new layers and means of storytelling, connects multiple museums worldwide, and that can be used remotely by anyone in the world.

1.8.3.3 3DINV workflow

**Description:** 3DINV application provides three-dimensional (3-D) inversion of surface Electrical Resistivity Tomography (ERT) data in order to automatically determine a 3-D resistivity subsurface model. The workflow comes in the form of a users’ manual which explains in detail how the software works.

1.8.3.4 AutoGR workflow

**Description:** AutoGR application is suited for large image datasets, such as the aerial photographs collected with UAVs or during systematic aerial surveys. The GRID system is going to speed up the georeferencing process. AutoGR can be used as online service for image georeferencing. The workflow is included in the users’ manual which explains in detail how the software works.

1.8.3.5 Dioptra workflow

**Description:** The metadata schema developed by the Science and Technology for Archaeology Research Center (STARC) has the goal to enable data interoperability and access to the digital resources stored in the local repository. Its structure allows retrieving models, activities, decision and answers the research question on how data can be used for data interpretation and re-used to perform further analysis and post-processing of raw data. The datasets stored in STARC repository refer to 2D and 3D cultural heritage data including archaeological sites, museum objects and architectonic elements. The schema is mostly based on LIDO and CARARE ones and is CIDOC-CRM compliant. The novelty of this metadata schema is the subset of metadata that has been designed to allow recording the information about the provenance of the digital objects, a particularly important aspect when the objects are 3D digital replicas of cultural objects. The workflow demonstrates how the metadata is applied.

1.8.3.6 CHERE workflow

**Description:** CHERE is used for documenting and streamlining operational procedures for management and use of cultural heritage data. Application enables efficient data creation and management for Institutions of culture as well as easier access to said data for general population. CHERE users’ manual contains workflows on how to install CHERE on your personal PC as well as how to use CHERE online.