Towards Model Execution Environment for Investigation of Heart Valve Diseases

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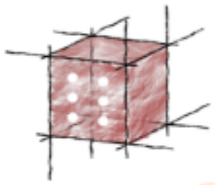


Outline

1. Motivation – personalized medicine; Virtual Physiological Human
2. Objectives
3. Data and computing flow
4. Model Execution Environment
5. File store
6. Integrated security
7. Visualization module
8. Summary

http://www.vph-institute.org/

In silico – turning big data into personalized medicine

11th October 2016

Room A8F388, European Parliament Brussels

15:00-17:00

15:00 – 15:05 Introduction by Co-chair

Nicola Caputo MEP (S&D, Italy)

15:05 – 15:25 "*in silico*, the digital age meets healthcare"

Professor Marco Viceconti - Executive Director INSIGNEO institute for in silico medicine, Sheffield University

15:25 – 15:45 "Turning aerospace software technology into solutions for healthcare"

Thierry Marchal - Industry Director for Healthcare, Construction and Consumer Products, Ansys

15:45 – 15:55: "Predictive models for medical devices"

Michael Hill - Vice-President for Science, Technology and Clinical Affairs, Medtronic

15:55 – 16:10: "A new model for the pharmaceutical industry"

Andrea Beccari - Drug Discovery Platform Manager, Dompé

16:10 – 16:30 FDA take on in silico – how do we regulate for the future?

Dr. Tina Morrison - Deputy Director, Division of Applied Mechanics at FDA

16:30 – 16:50 Discussion period

Moderated by Alison Abbott – Nature Magazine

16:50 – 17:00 Closing remarks and conclusions

Seán Kelly (EPP, Ireland)

17:00 Drinks Reception

**5 min Q&A after each presentation*

Atmosphere Cloud Platform

VPH-Share Master Interface host
portal.vph-share.eu

Cloud Management Portlets

Provide GUI elements which enable service developers and end users to interact with the Atmosphere platform and create/deploy services on the available cloud resources

Secure RESTful API (Cloud Facade)

WP2 Core Services Host
vph.cyfronet.pl

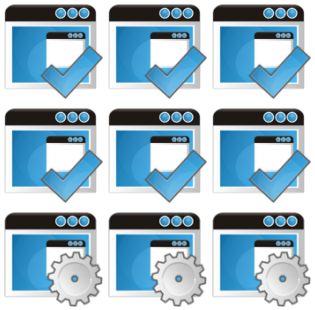
Atmosphere Core

- Authentication and authorization logic
- Communication with underlying computational clouds
- Launching and monitoring service instances
- Creating new service templates
- Billing and accounting
- Logging and administrative services

Atmosphere Registry (AIR)

user accounts

available cloud sites



services and templates

Head Node

Image store

Worker Node

96 CPU cores

184 GB RAM

4 TB storage

private IP space

VPH-Share cloud site at ACC CYFRONET AGH

Head Node

Image store

Worker node w/large resource pool („fat node")

128 CPU cores

256 GB RAM

4 TB storage

private IP space

VPH-Share cloud site at UNIVIE

API host

Image store

Worker Node

Massive (functionally limitless) hardware resource pool

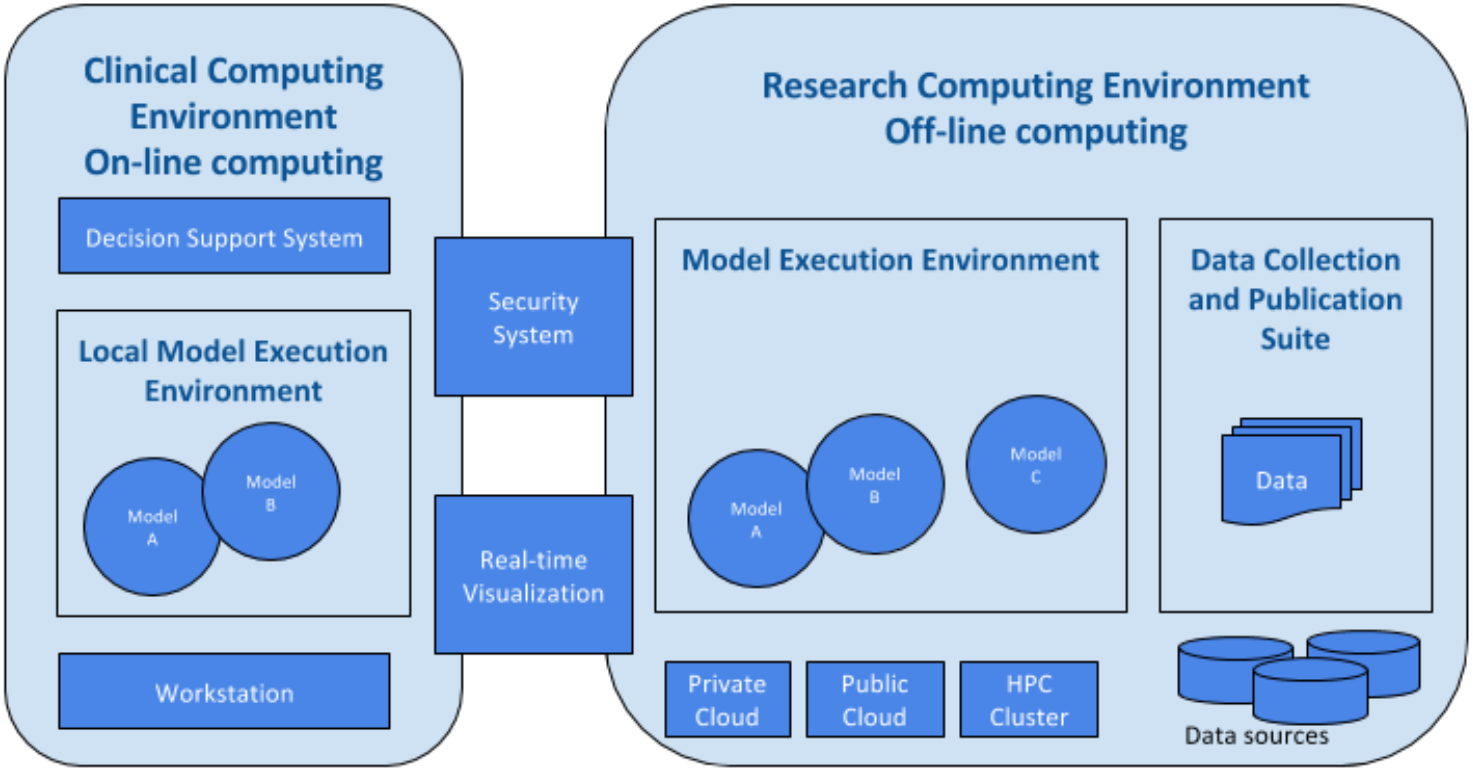
public IP space

Amazon Elastic Compute Cloud (EC2) – European availability zone

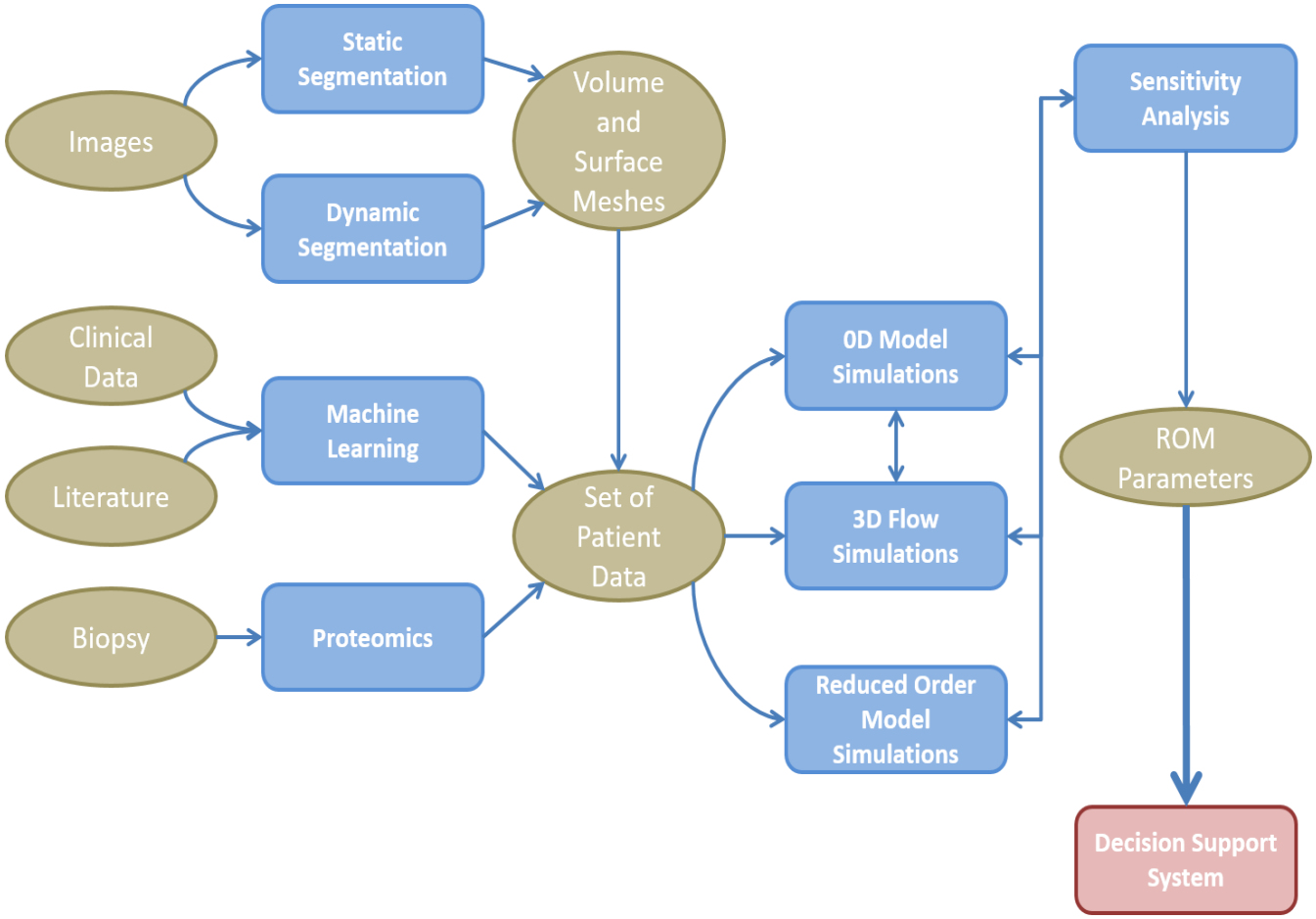
Motivation

- Investigations leading to practical implementations of personalized medicine are challenging
- The main goal of the EurValve project is to combine a set of complex modeling tools to deliver a workflow which will enable evaluation of medical prospects and outlook for individual patients presented with cardiovascular symptoms suggesting valvular heart disease
- This research should result in a decision support system (DSS) which can be applied in clinical practice
- This research activity requires a dedicated problem solving environment which we refer to as the Model Execution Environment (MEE)

DSS and Research Environment



Data and action flow



Data and action flow consists of steps involving image segmentation, proteomics analysis and literature mining to construct system models which, in turn, enable building reduced order models as the knowledge base for the DSS.

Objectives

To develop and provide the necessary infrastructure to:

- Collect, represent, annotate and publish core homogeneous data
- Store and give secure access to the participating clinical centres and to the development partners to the necessary data
- Execute the models in the most appropriate computational environment (private workstation, private cloud, public cloud) according to needs
- Support real-time multiscale visualisation.

To develop an integrated security system supporting:

- Authentication and authorisation
- Data encryption for secure processing in public clouds

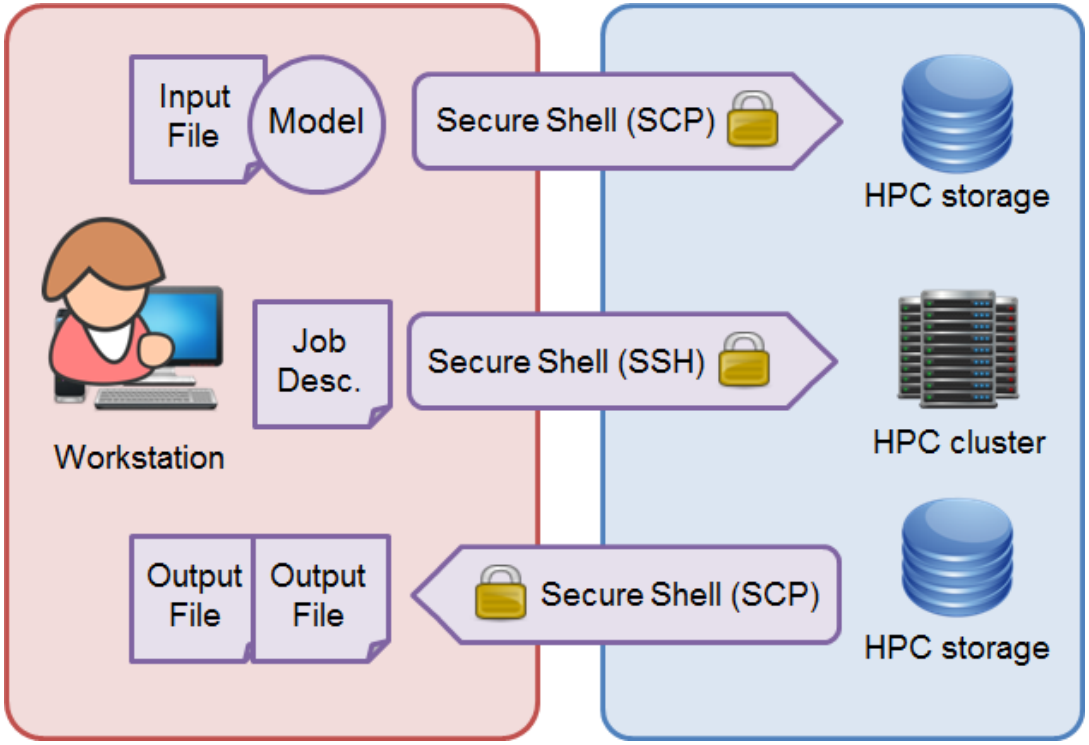
To deploy and operate the developed infrastructure, ensuring:

- Quality of software components deployed and installed
- Quality of service, including such aspects as availability, responsiveness and cost efficiency

Examples of user requirements

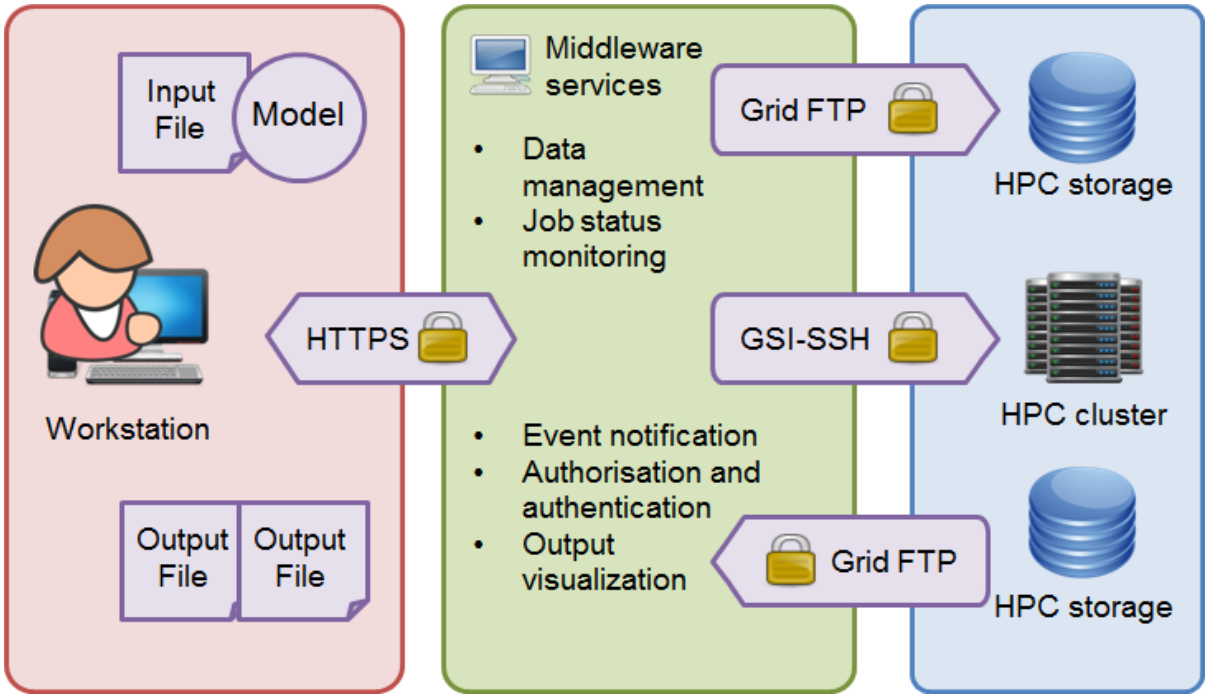
1. Execution environment delivers access to commercial numerical computing environments such as Matlab and AnsysCFD solvers (it will be used to deliver 0D system model and ROM creation of 4D CFD)
2. Execution environment delivers access to significant computer power and storage (ROM creation requires a lot of computer power and storage, >1000 CPU, many TB of HDD)
3. Some of the computations will be executed outside the research environment (e.g. Segmentation will be run locally with node-locked license)
4. Data is transferred from data warehouse to compute environment
5. Sensitivity analyses are visualized while the computation takes place
6. The environment should support interactive and batch processing
7. Interaction with selected services should be automated by scripting or Web UI interfaces

Basic mode of access to HPC



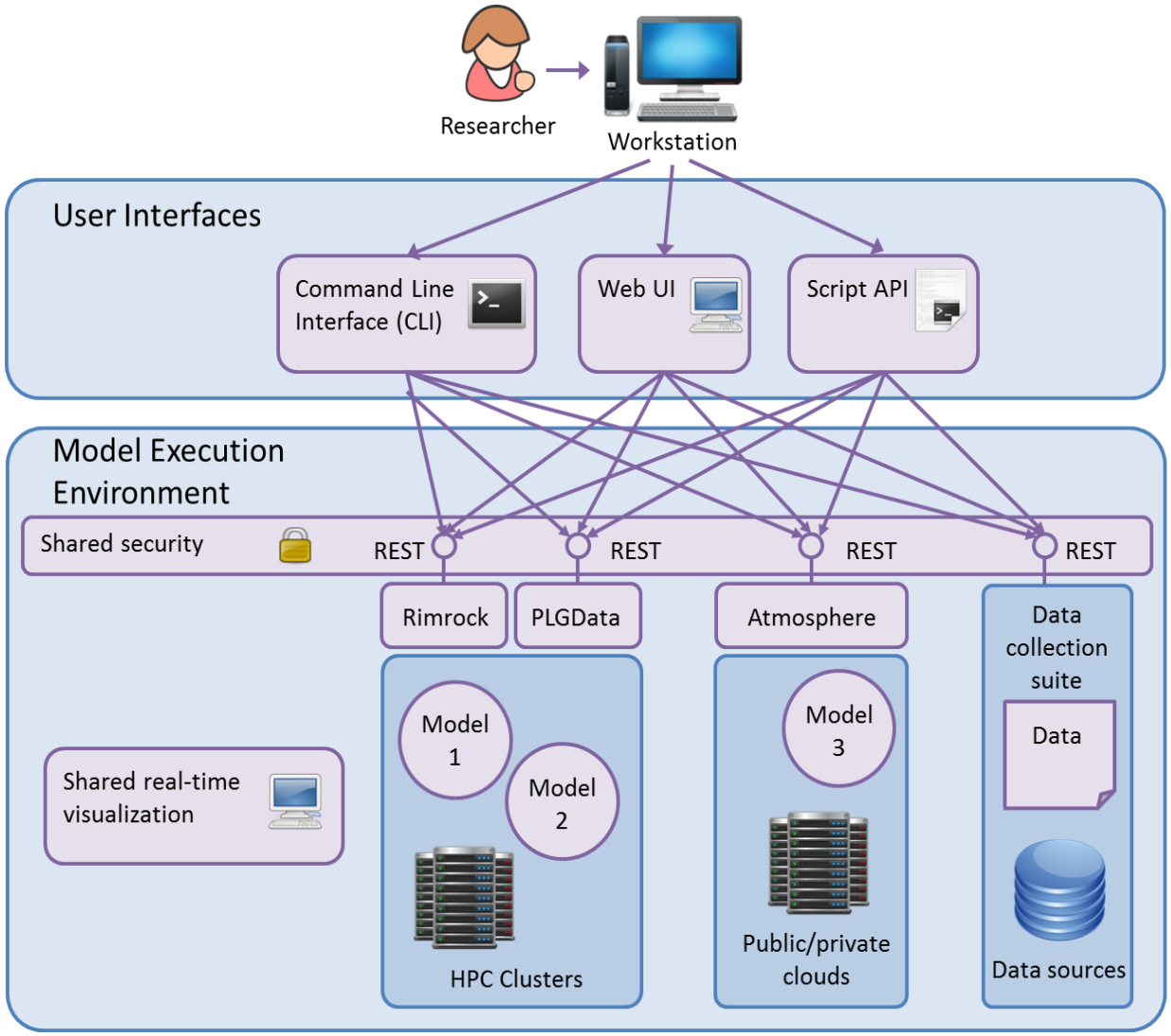
A user, utilizing a series of secure shell connections, transfers files (e.g., simulation input files, heart valve 3D model) to the HPC cluster's file system, submits a computational job execution (for instance, a fluid dynamics simulation) and retrieves job execution output (e.g., the visualization of the performed blood flow simulation through the uploaded heart model).

Middleware based access to HPC



The user delegates one's credentials to middleware services, which in turn manage user's input and output data, create and submit the computational job description, actively monitor job execution on the remote computational cluster, and notify the user of completion status. Sometimes such services are also able to visualize simulation execution outputs to the user.

Vision: Model Execution Environment



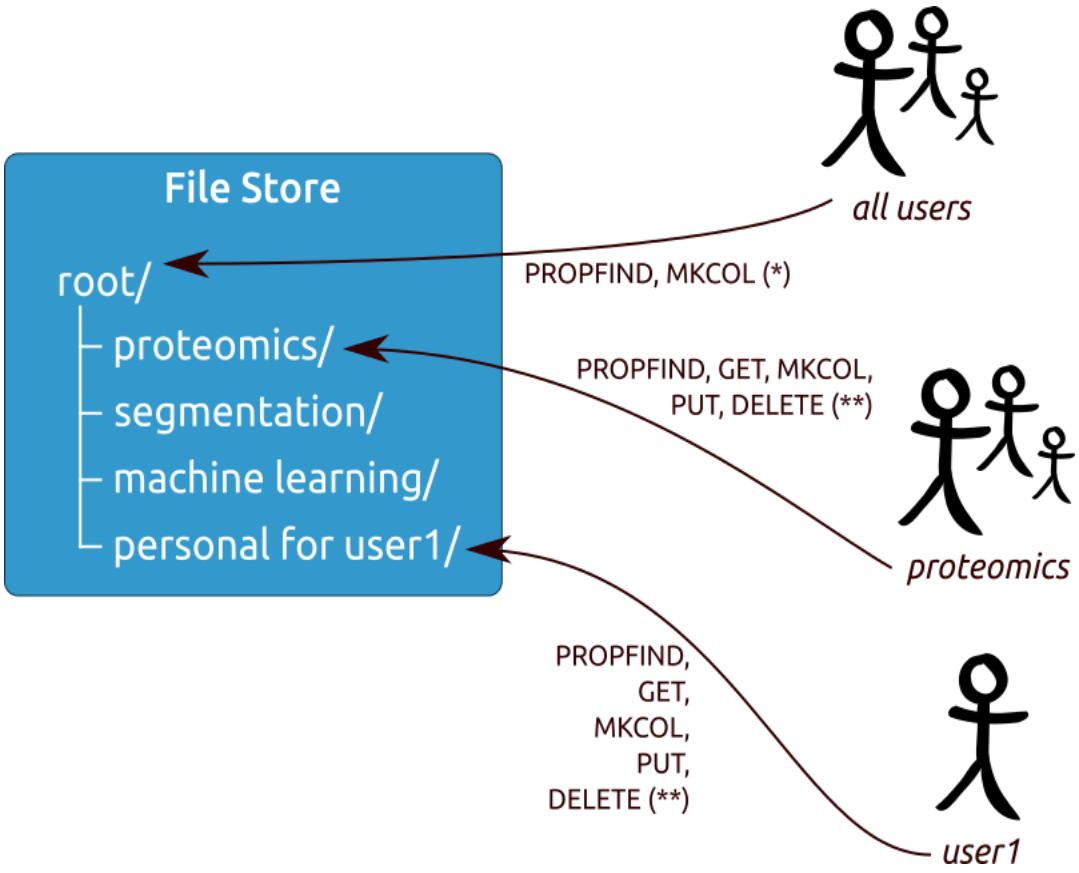
Alpha version of MEE – 3 services

- **EurValve File Store - https://files.valve.cyfronet.pl**
- **EurValve Portal - https://valve.cyfronet.pl**
- **Security subsystem**

EurValve File Store

- Deployment of a file repository compliant with the WebDav protocol, including search capabilities (RFC 5323)
- Modification and integration of the FileStore component (developed within VPH-Share) allowing for web-based file browsing/downloads/uploads as part of the newly created EurValve portal
- Securing the file repository with a EurValve's security compatible mechanism

File Store - multi policy approach



Access policies are attached to different nodes according to user sharing actions.
Private spaces can be created for individual users and groups.

Model Execution Environment Prototype

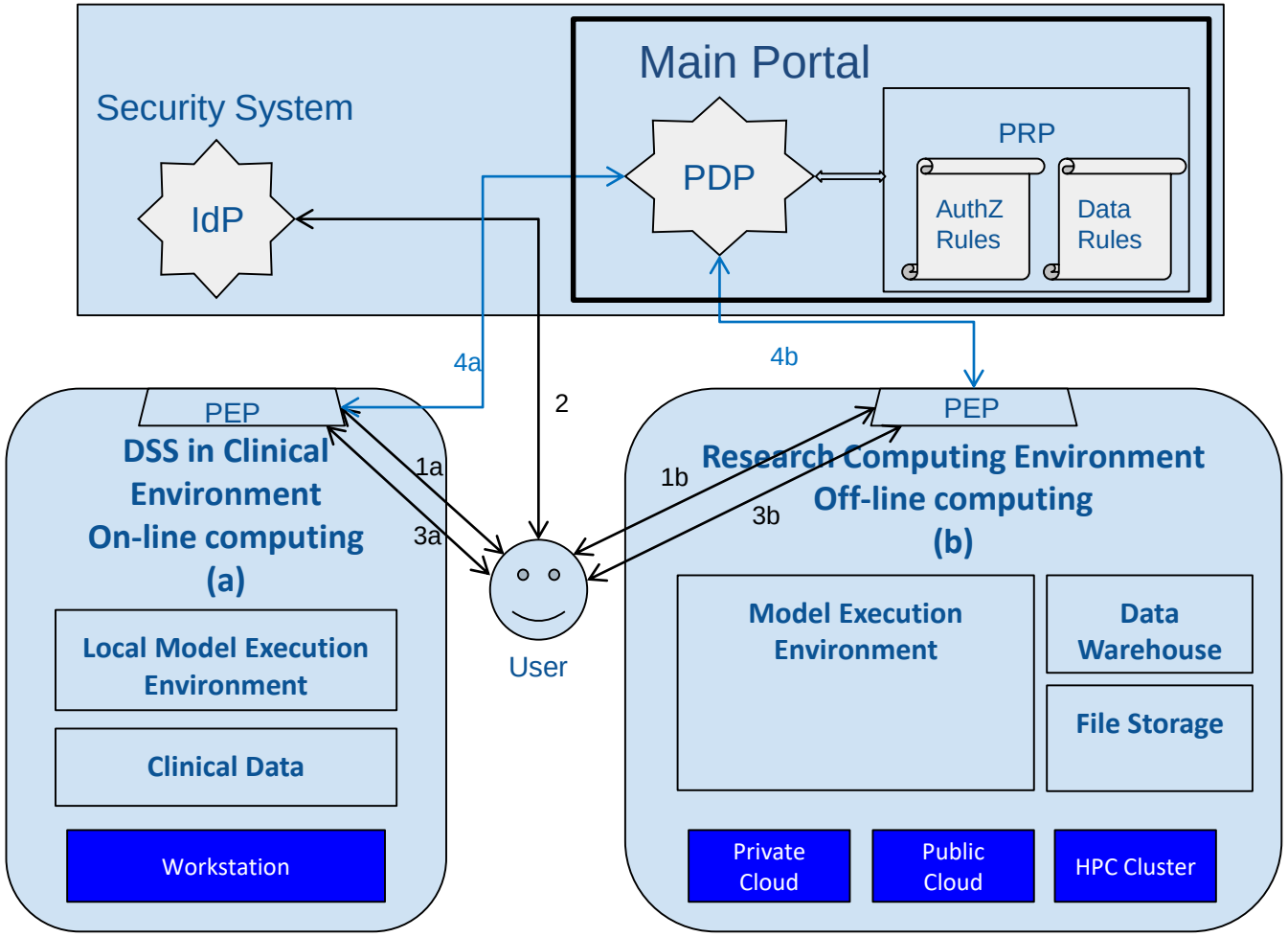
Components

- Valve portal – discover collected files for patient clinical case, submit blood flow computation into Prometheus supercomputer, monitor computation execution, discover results
- Rimrock – tool for submitting jobs into Prometheus supercomputer
- PLData – web based file browser for Prometheus files
- Prometheus supercomputer

Typical use case

1. Create new Patient clinical case
2. Discover files connected with the Patient
3. Run blood flow computation on Prometheus supercomputer
4. Monitor computation execution
5. Discover produced results and update clinical case progress

Integrated Security and Data Protection



- **Step 1-2**: Users authenticate themselves with the selected identity provider (hosted by the project or external trusted one) and obtain a secure token which can then be used to authenticate requests in DSS and RCE.
- **Step 3-4**: Authorization to use computational services is granted in accordance with policies stored in PDP. Optionally user may request service access from resource manager.

IdP - Identity Provider
PDP - Policy Decision Point
PRP - Policy Retrieval Point
PEP - Policy Enforcement Point

PDP, PEP – typical use case

Components

- PDP – policy decision point implemented as Valve Portal REST interface
- UI to configure permissions for concrete resource. Permission can be given for concrete user or for the group of users
- PEP – policy enforcement point implemented as Nginx module

Use case

1. A request without JWT (JSON web token) is made to a service secured by PEP – the unauthorized response code is returned (401)
2. A request accompanied by a valid JWT is made, resulting in an access denied (403) exception
3. Another user registers a service and authorizes other users to access it
4. The procedure performed in step 2 is repeated – this time permission is granted (200) and secured content is returned to the user

File Store typical use case

Components

- UI to facilitate user login and data store access
- Authentication mechanisms
- PDP, PEP – policy decision/enforcement point to grant/revoke access to resources on the basis of resource owners' decisions

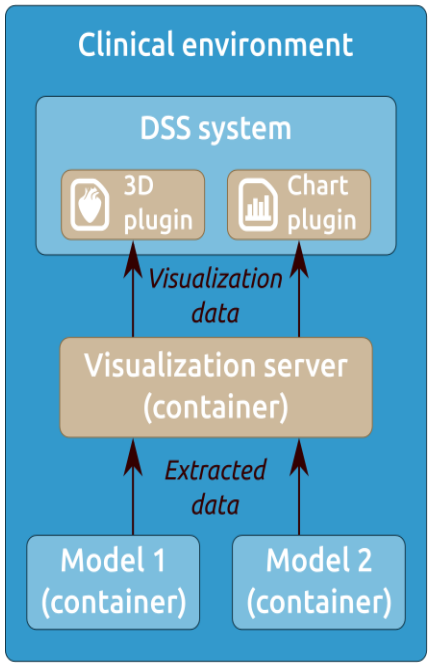
Scenario

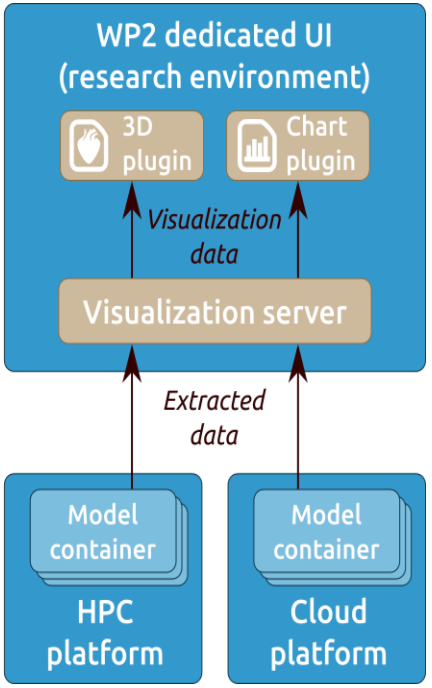
1. User 1 logs into the UI, accessess the File Store component and creates a directory
2. User 1 uploads a file to the newly created directory
3. User 2 logs in and attempts to retrieve the file – however, directory access is denied due to lack of sufficient permissions.
4. User 1 grants User 2 read-only access for the newly created directory
5. User 2 is now able to enter the directory and retrieve its content. He is, however, unable to upload new files due to the lack of „write" permissions.
6. User 1 extends User 2's permission set with „write" access.
7. User 2 is now able to create new files and subdirectories in the target directory.

Real-time Multiscale Visualization

Deployment to local and remote Model Execution Environments

- Using container technology for packaging
- Integration with HPC, local and research computing infrastructure
- Visualization components available as embeddable web browser views





MEE services at Cyfronet (alpha versions)

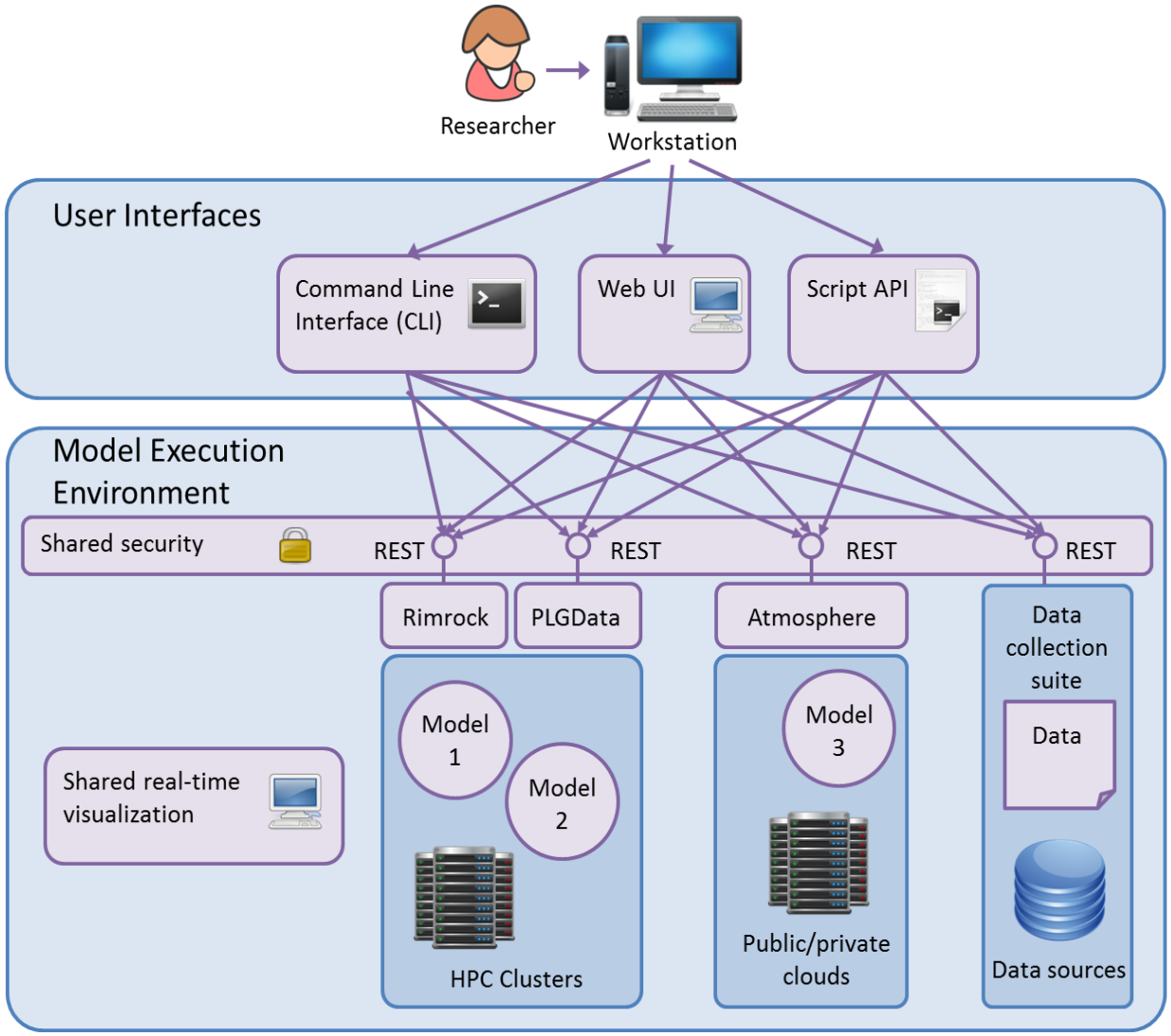
- **EurValve Portal**
  - URL: https://valve.cyfronet.pl
  - Registration at: https://valve.cyfronet.pl/users/sign_up

- **EurValve File Store**
  - URL (docs): https://files.valve.cyfronet.pl
  - WebDAV endpoint (portal account required): https://files.valve.cyfronet.pl/webdav

Summary

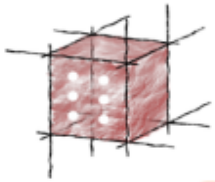
- Detailed requirements formulated and state-of-the-art in the area of valvular diseases analyzed
- Detailed design recommendations relating to model-based research environments established
- Prototypes of the Model Execution Environment, with supporting File Store and Integrated Security components facilitating simulations with the aim to develop decision support systems for heart diseases

Towards Complete Model Execution Environment



H2020 Project 689617: EurValve

http://www.eurvalve.eu



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