EurValve Model Execution Environment in Operation

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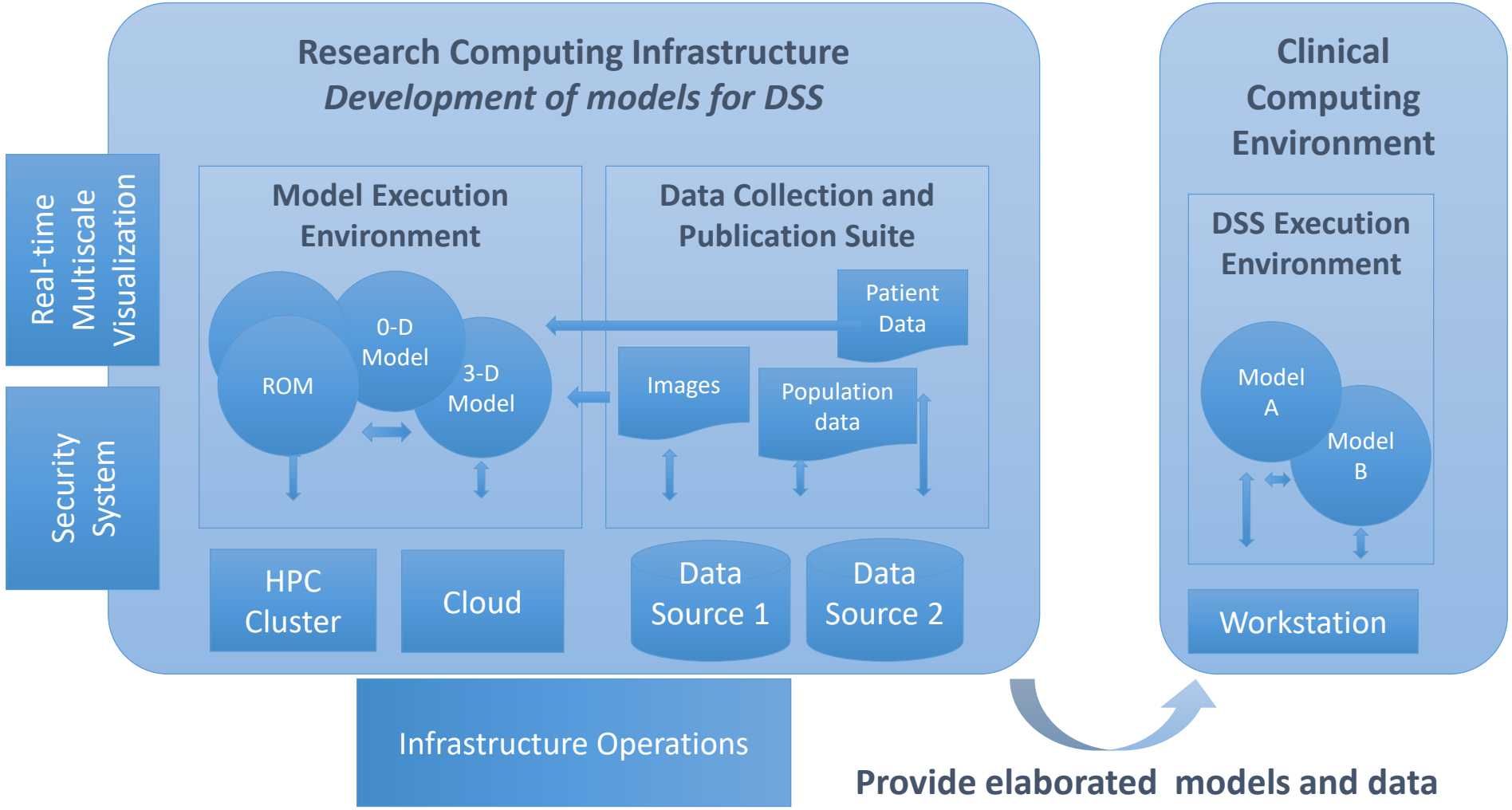
Outline

- Motivation: towards a Decision Support Systems for valvular deseases
- Requirements for computing and storage
- Architecture of the Model Execution Environment
- Implementation of the Model Execution Environment
- MEE in operation: a patient pipeline
- Recorded demos of MEE operation
- Summary and future work

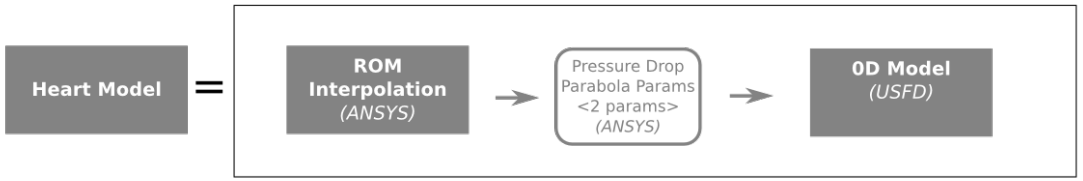
From Research Environment to DSS

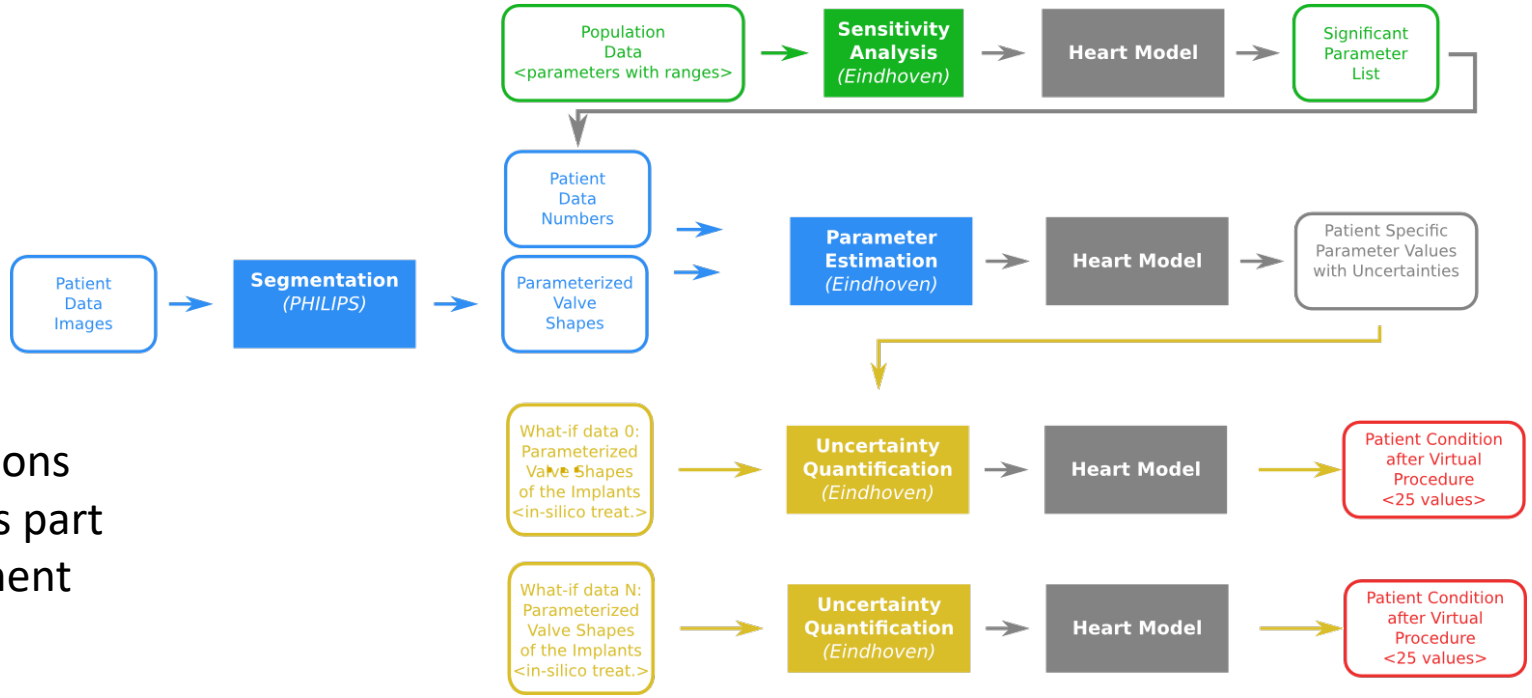


Pipelines for ROM and sensitivity analysis

Data and action flow consists of:

- full CFD simulations
- sensitivity analysis to acquire significant parameters
- parameter estimation based on patient data
- uncertainty quantification of various procedures



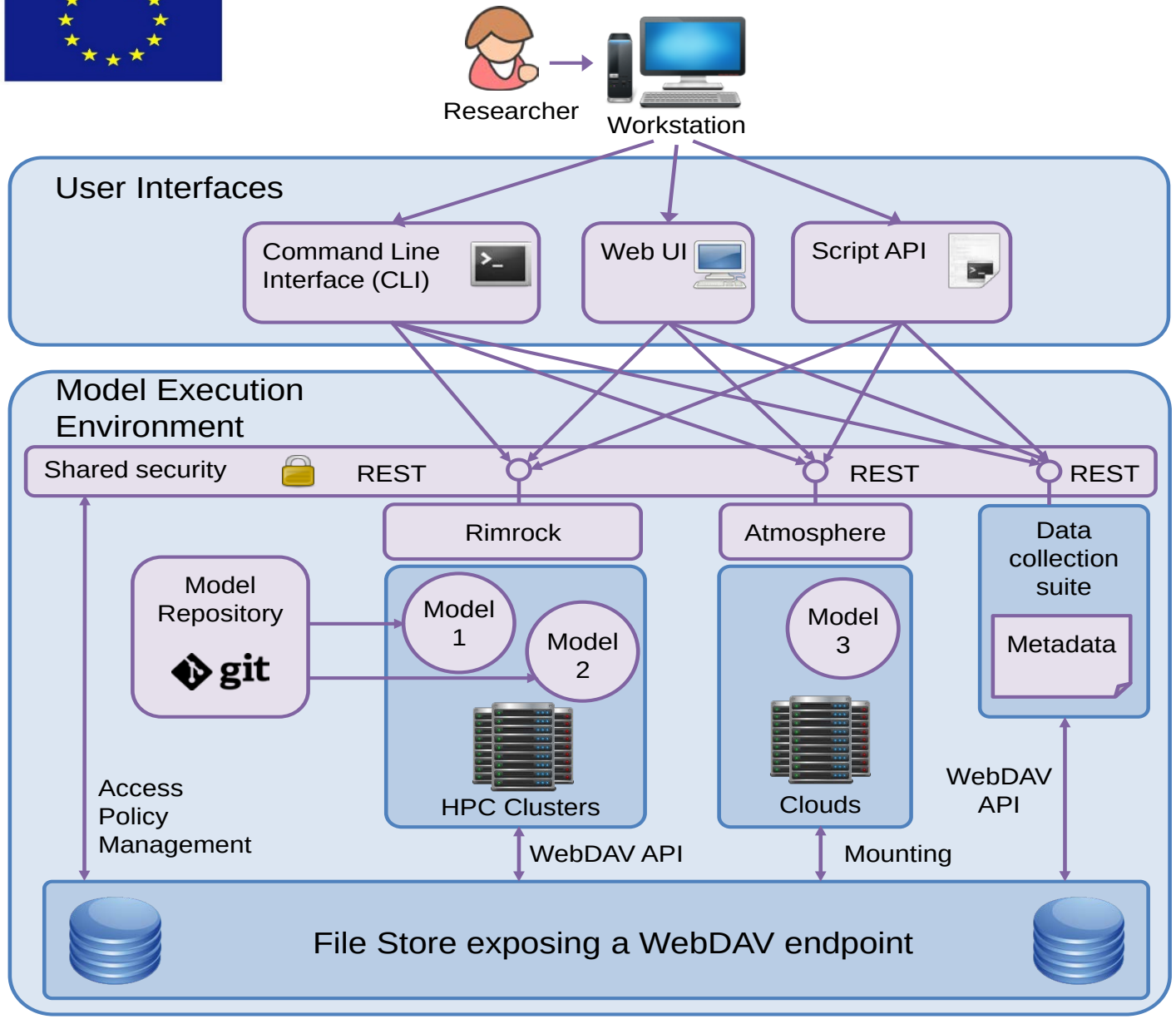


The flow of CFD simulations and sensitivity analysis is part of clinical patient treatment

Functionality of Model Execution Environment

- Reproducibility, versioning, documentation of the pipeline
- Automation of the simulation pipeline with human in the loop for:
  - new models, new versions of models,
  - new users
- Data preservation
- Basic provenance features
- Helpful visualization of simulation flow and obtained results
- Generation of some components of publications
- Portability

Model Execution Environment - structure



- The MEE can be interfaced from a dedicated GUI (the EurValve Portal), through a RESTful API or through a comman-line interface, depending on the researcher's preferences.
- Computational tasks can be run on HPC resources or in a cloud environment, as appropriate.
- A uniform security layer is provided.

API – Application Programming Interface

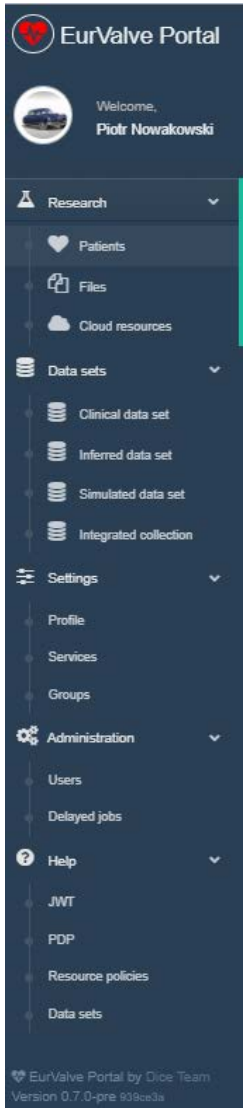
REST – Representational state transfer

Rimrock – service used to submit jobs to HPC cluster

Atmosphere – provides access to cloud resources

git – a distributed revision control system

Implementation of MEE



Model Execution Environment:

- Patient case pipeline integrated with File Store and Prometheus supercomputer
- *File Store for data management*
- Cloud resources based on Atmosphere cloud platform

Data sets

- Structural access to patient databases
- Query interfaces for real, simulated and inferred data

Security configuration

- Service management – for every service dedicated set of policy rules can be defined
- User Groups – can be used to define security constraints

REST API

- Creating a new user session – as a result, new JWT (JSON Web Token) tokens are generated for credential delegation
- PDP – Policy Decision Point: check if user has access to concrete resource
- Resource policies – add/remove/edit service security policies

MEE extensibility – support for additional computational modules

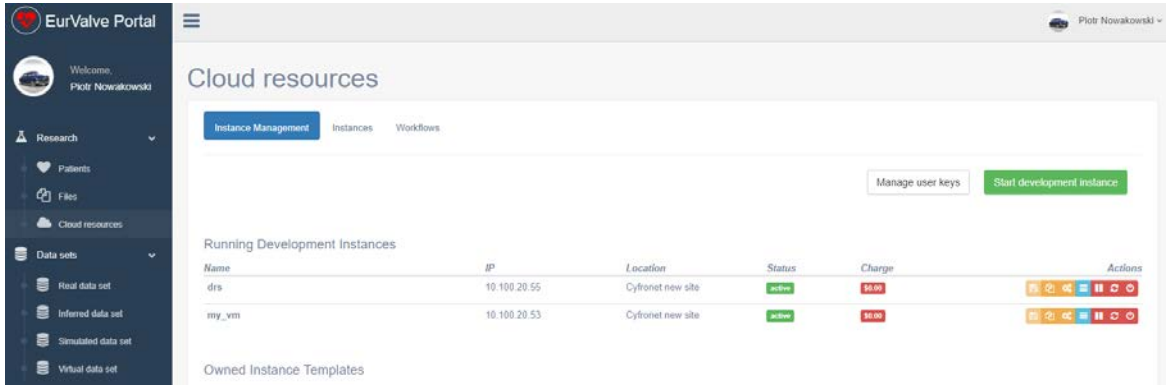
Additional modules can be implemented:

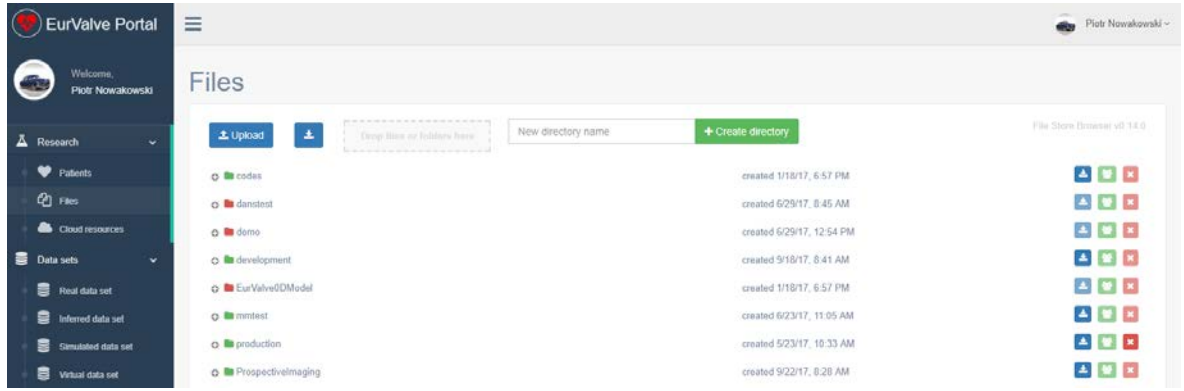
- As applications deployed on the Prometheus supercomputer
- As external services communicating with the platform via its REST interfaces
- As virtual machines deployable directly in the Cyfronet cloud via the Atmosphere extension of the MEE

Encapsulating pipeline steps as HPC tasks:

- Scripts are run on the Prometheus supercomputer via the Rimrock extension
- Files uploaded to the FileStore (e.g. using MEE GUIs) can be accessed on Prometheus nodes via **curl**, leveraging the WebDAV interface provided by FileStore
- Any result files can also be uploaded directly to FileStore from the Prometheus computational nodes
- External tools can be used to monitor job completion status e.g. by periodically scanning FileStore content

Generic MEE tools





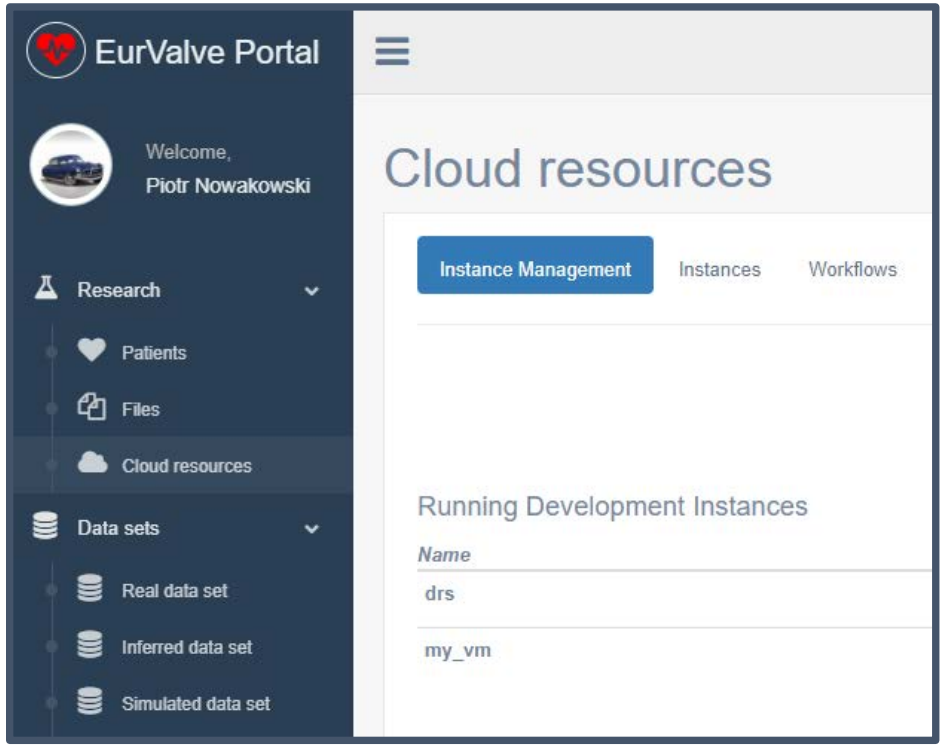
Cloud resources

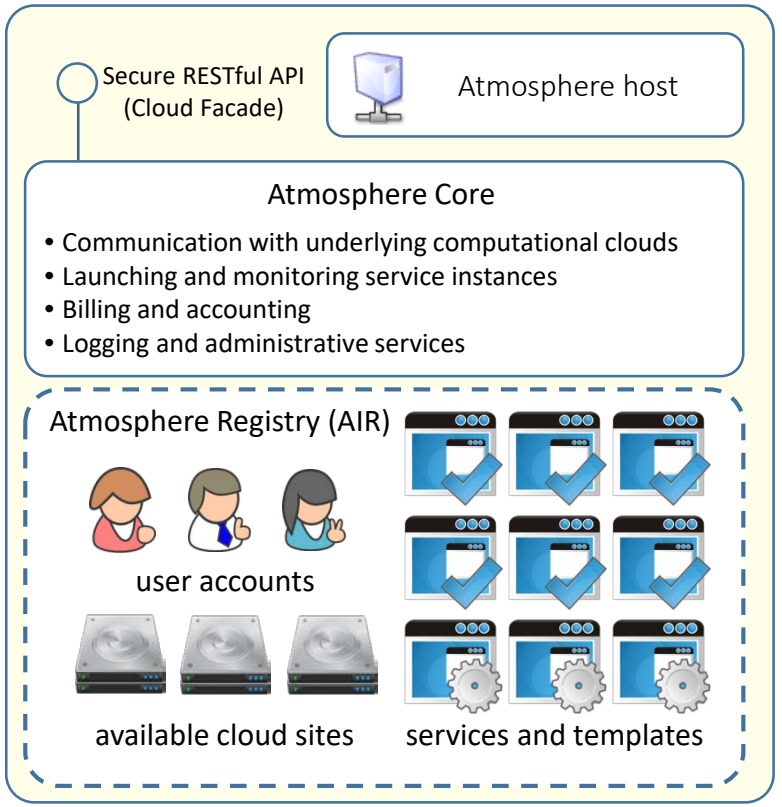
- Based on Atmosphere cloud platform
- Can start/stop/suspend virtual machine on cloud infrastructure
- Can save running existing machine as template
- (Future) can share templates with other users

File Store

- Basic file storage for the project
- Ability to create new directories and upload/download files
- Can share directories with other users or groups of users
- Can be mounted locally using WebDav clients
- The File Browser GUI can also be embedded in other views

MEE - cloud access via Atmosphere

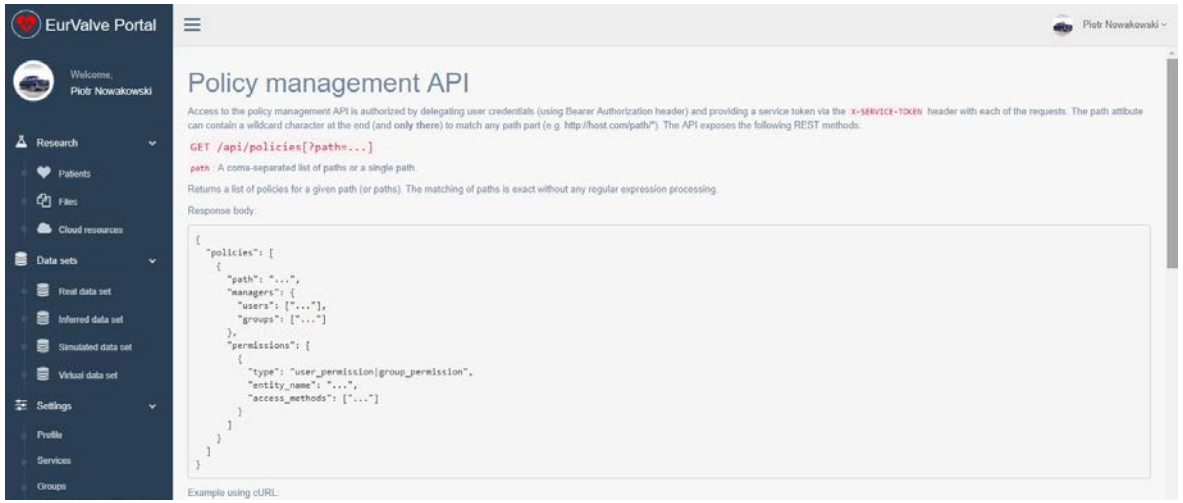




Access to cloud resources

- The Atmosphere extension provides access to cloud resources in the EurValve MEE
- Applications can be developed as virtual machines, saved as templates and instantiated in the cloud
- The extension is available directly in the MEE GUI and through a dedicated API
- Atmosphere is integrated with EurValve authentication and authorization mechanisms

MEE functionality via REST API



Generate user JWT Token

- User (or other service) can retrieve new JWT token by passing username and password
- JWT token can be used for user credential delegations by external EurValve services

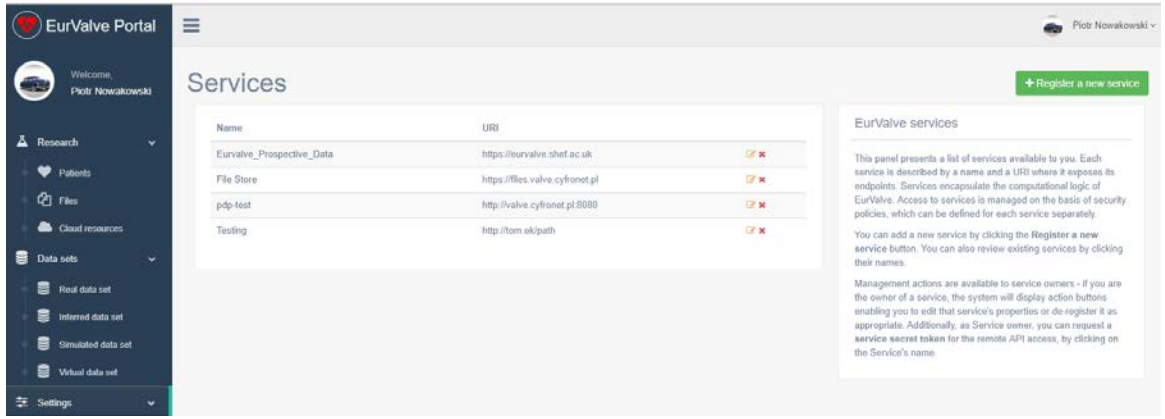
PDP API

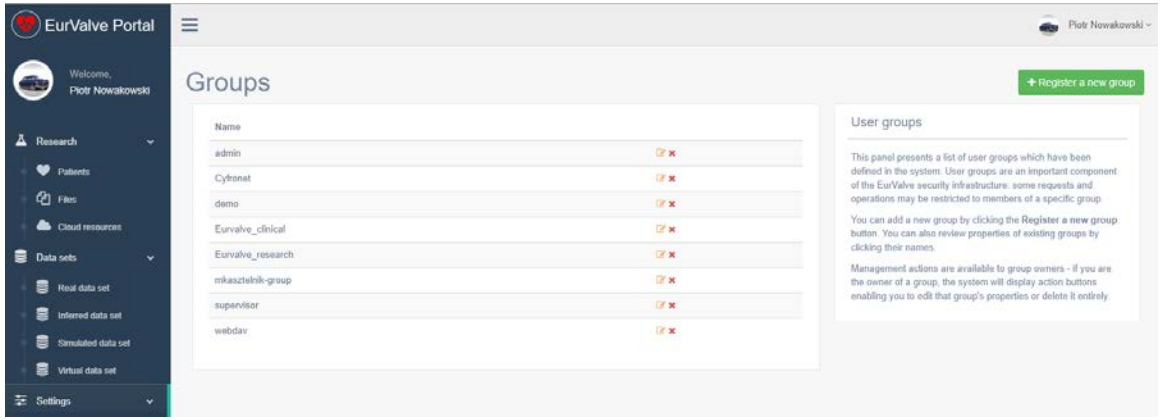
- Check if user has right to access a specific resource

Resource policy management

- Create/edit/delete local policies by external EurValve service on user behalf
- Currently integrated with File Store
- Initial ArQ integration tests underway

MEE security management UIs





Services

- Basic security unit where dedicated security constraints can be defined
- Two types of security policies:
  - Global – can be defined only by service owner
  - Local – can be created by the service on the user's behalf

Groups

- Group users
- Dedicated portal groups:
  - Admin
  - Supervisor – users who can approve other users in the portal
- Generic groups:
  - Everyone can create a group
  - Groups can be used to define security constraints

Recorded demos of MEE

- Logging in to EurValve and PLGrid systems – https://youtu.be/4I907aAOCvU
- File Store Browser – https://youtu.be/-6fXG0am6iE
- Distributed Cloud File Store – https://youtu.be/FTF-QaI5ZZQ
- Services, security, restricted access – https://youtu.be/-6fXG0am6iE
- Cloud Resource Access – https://youtu.be/A4wkxFCRLak
- Patient case
  - https://youtu.be/SIwpxdoQYWw (patient case)
  - https://youtu.be/j0Nu-E-0elE (pipeline diff)
- Integration of computational services – https://youtu.be/SIwpxdoQYWw

The Patient Case Pipeline

1. Segmentation – to start this calculation, a zip archive with a dedicated structure needs to be created and transferred into the OwnCloud input directory. Next, the output directory needs to be monitored for computation output.
2. Reduced Order Model analysis – based on the results of the segmentation step, a ROM simulation is executed and its results uploaded to the File Store.
3. Parameter Optimization – a technical step which prepares suitable parameters for the 0D model sequence
4. 0D model sequence – runs four versions of the 0D model analysis for various input datasets
5. Uncertainty Quantification – Matlab script which can include the 0D Heart Model. It will be executed on the Prometheus supercomputer, where input files will be transferred automatically from the File Store. Results are transferred back from Prometheus to the File Store.
6. Output visualization – produces actionable visualization of the 0D model output data based on File Store contents.

Patient Case Pipeline high-level building blocks:

- File-driven computation (such as Segmentation) – use case: upload file to remote input directory, monitor remote output directory for results
- Scripts started on Prometheus supercomputer – use case: transfer script and input files from File Store to the cluster, run job, monitor job status, once the job has completed – transfer results from the cluster to File Store (examples: 0D Heart Model, Uncertainty Quantification, CFD simulation)

Future work

1. Further improvement of the MEE based on user feedback
2. Implementation of computation quality validation against retrospective patient data in order to compare pipeline results with retrospective patient data measured *in vivo* following intervention
3. Implementation of additional automation features for existing pipelines, enabling fine-grained control over the configuration and execution of individual pipeline steps in the context of specific patient data.
4. Development of advanced accounting mechanisms:
   - logging events, such as data access or attempts to do so, with appropriate metadata
   - analysis of events to detect anomalies (such as suspected access from new IP/location, device etc.) to potentially alert administrators, data owners, users etc. about suspicious activities.

More at

http://dice.cyfronet.pl

http://www.eurvalve.eu

EurValve H2020 Project 689617