Data access and integration in a distributed computational environment for medical research

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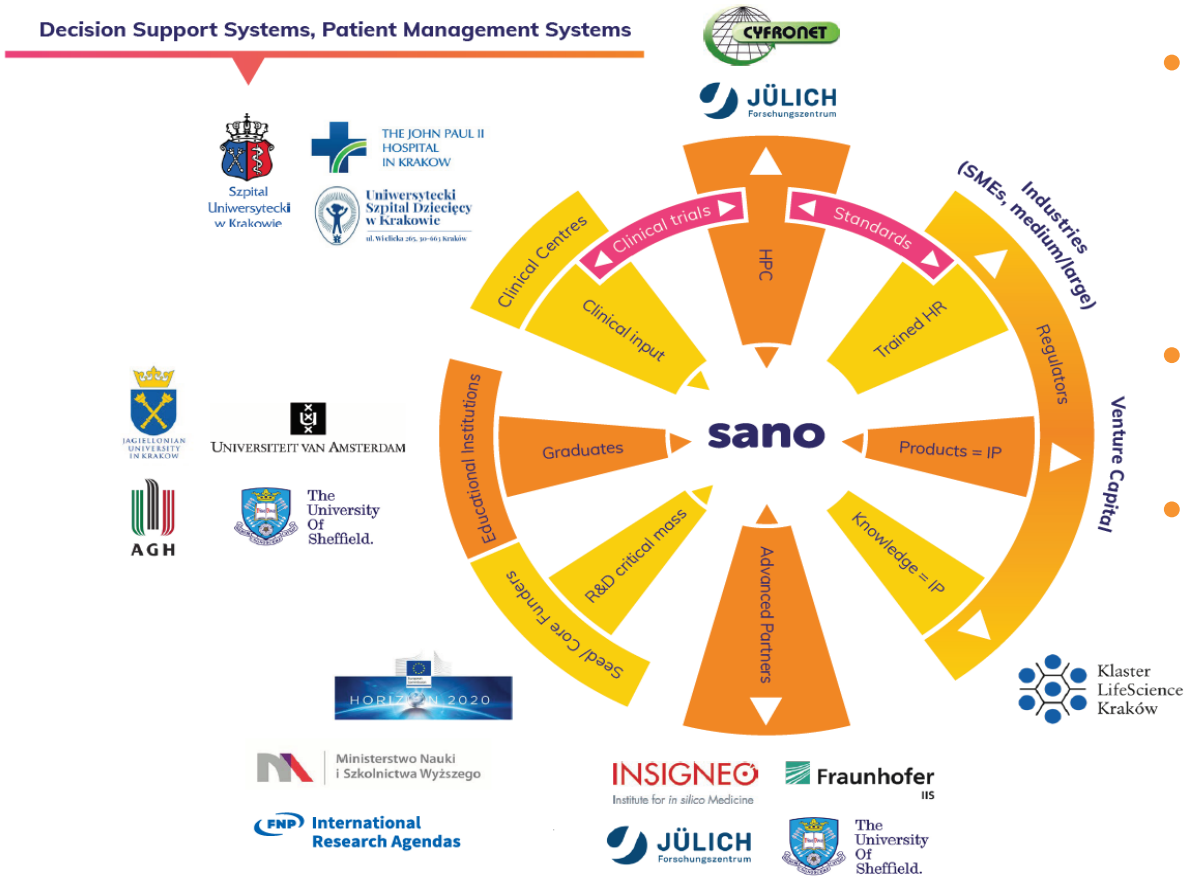
Overview

- *Introduction to the mission of Sano*
- *The Sano computational toolkit – tools and services*
- *Research initiatives*
- *Data access challenges*
- *Closing remarks*

Sano at a glance



- Sano – Centre for Personalised Computational Medicine – has been founded as a Centre of Excellence in development and deployment of decision support systems in medical science
- The Centre is based in Kraków, Poland, and operates as an independent foundation
- The Centre's activities involve integrating and processing large volumes of data related to medical research and decision support

https://sano.science

Sano - technical infrastructure

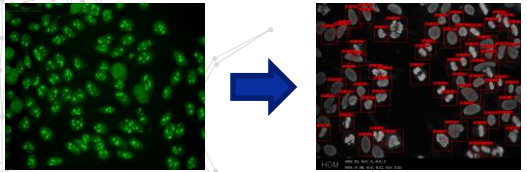
The Centre will support the work of **six independent research teams**, *each headed by a Research Team Leader and focusing on a specific area of computational medicine, as defined in Sano's International Research Agenda*

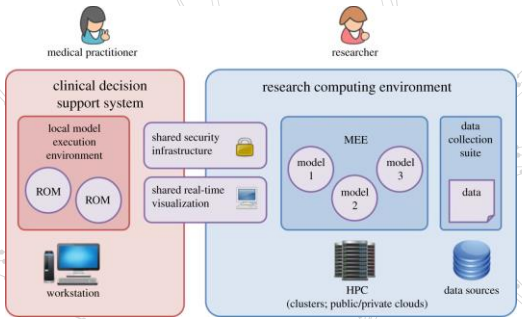
Sano provides general hardware and software infrastructure in support of collaborative R&D work:

- **Compute time:** *HPC grants: currently 300k CPU-hrs + 100k GPU-hrs*
- **R&D support staff:** *currently 6 part-time employees: ICT service team/Scientific Programmers team*
- **Software for code development:** *workflows, versioning, code audits*
- **Website:** *hosting and backup in Poland*
- **Basic hard- and software:** *notebooks, e-mail, cloud storage*

Initial Research Projects at Sano

- *Funded by IRAP Plus (Foundation for Polish Science)*
- *Goal: building research capacity, establishing collaborations via Sano*
- *Examples of collaborative projects initiated:*
  - *Image classification for immunological diseases (collaboration with CMUJ)*
  - *Modelling and simulation of Pulmonary Hypertension in (collaboration with USFD)*
  - *Feature selection for multiclass classification (collaboration with OMICRON UJ and Biobank Lab Univ. of Lodz)*
  - *Statistical methods of Machine Learning for Vasculitis (collaboration with CMUJ)*





Tools and Services

As part of its mission, Sano provides researchers with access to a comprehensive computational toolkit, including documentation and support staff

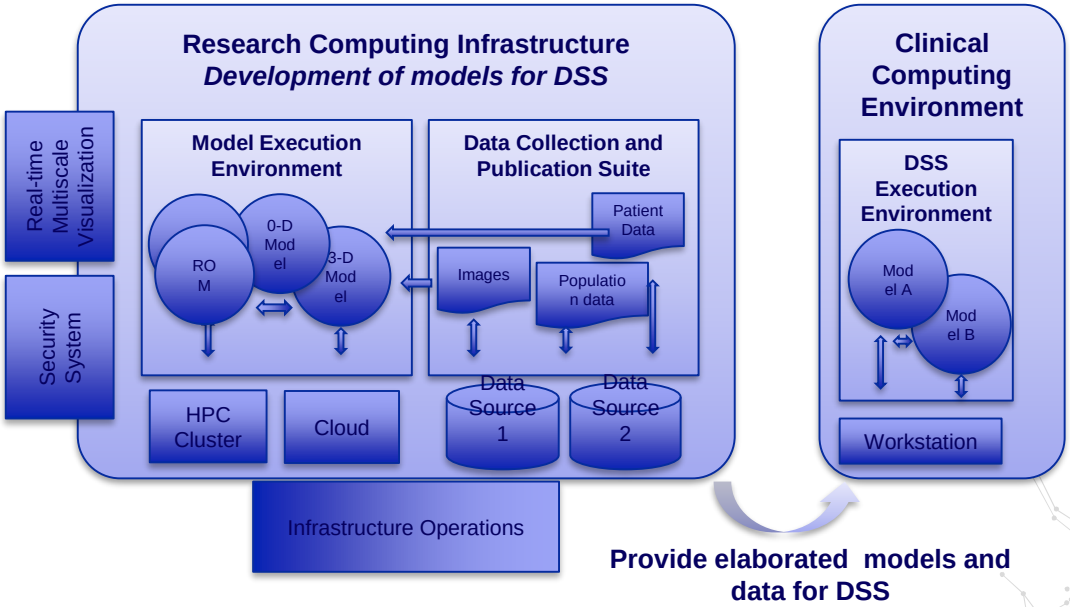
- **PLGrid access:** *user registration and certificate issuing in place – enables free-of-charge use of PLGrid resources, including a variety of proprietary (licensed) software, such as CFD solvers, Matlab, other specialized packages*
- **Model Execution Environment (MEE):**
  - *Comprehensive platform for deployment and reuse of computational models*
  - *Enables scientific computational pipelines running on HPC devices*
- *PLGrid also provides* **Virtual Machines** *for individual research tasks*

Challenge: how to integrate all of the available infrastructure into a coherent platform upon which large-scale (and medium-scale ;) scientific simulations can be executed in a secure, repeatable fashion?

Data access challenges at Sano

- Ensuring that data can be brought to where computations are performed – requires mechanisms for moving large data packets around the distributed environment
- Anonymization and secure storage of medical data sets (with GDPR compliance)
- „Right to be forgotten” – how to ensure that data is erased when the Centre no longer has permission to process it
- Easy upload and retrieval of input data and results to/from HPC platforms (which often do not provide convenient GUIs for end users)

Model Execution Environment – a computation and data integration platform

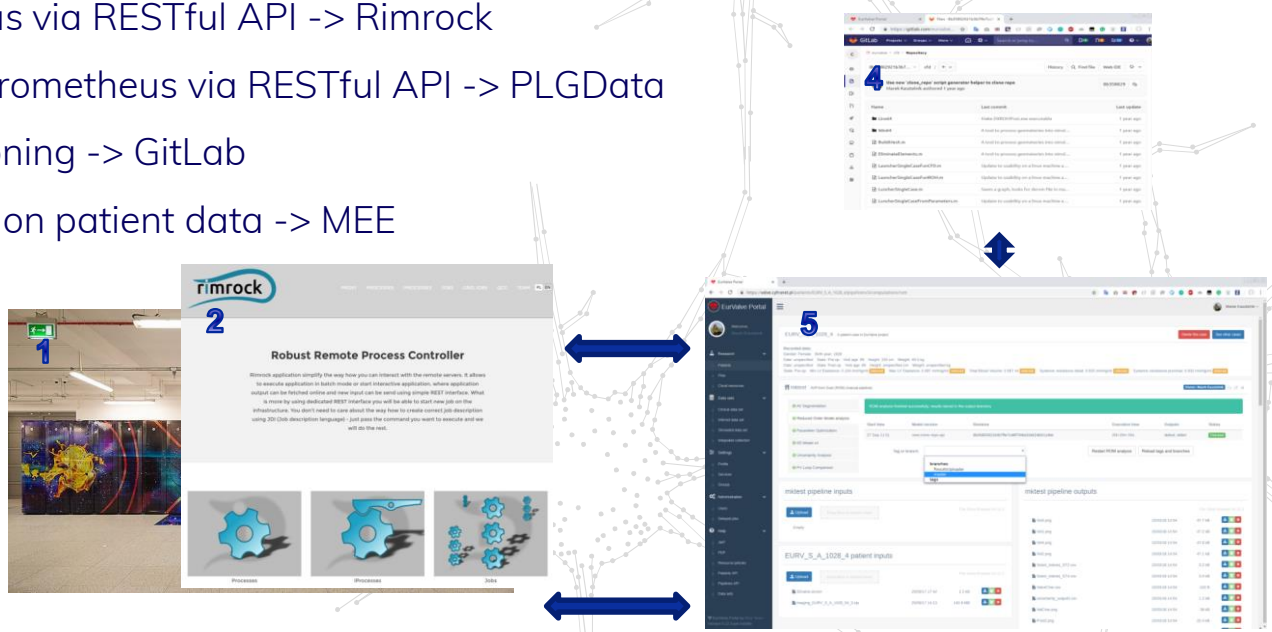


- The genesis of MEE dates back to the EurValve project, which called for extensive processing of large amounts of experimental data in order to prepare a data set which would later enable the operation of a clinical decision support system (DSS)
- The data concerned patients with valvular heart disease, and the goal of the DSS was to supply recommendations regarding their treatment
- Due to the fact that the DSS could not directly rely on HPC capabilities, heart models had to be precomputed in advance, by domain scientists (cardiologists)
- Thus, an environment was needed which would facilitate this task without requiring in-depth IT knowledge
- In addition to enabling execution of computational model on HPC resources, the tool called for integration of various data storage resources

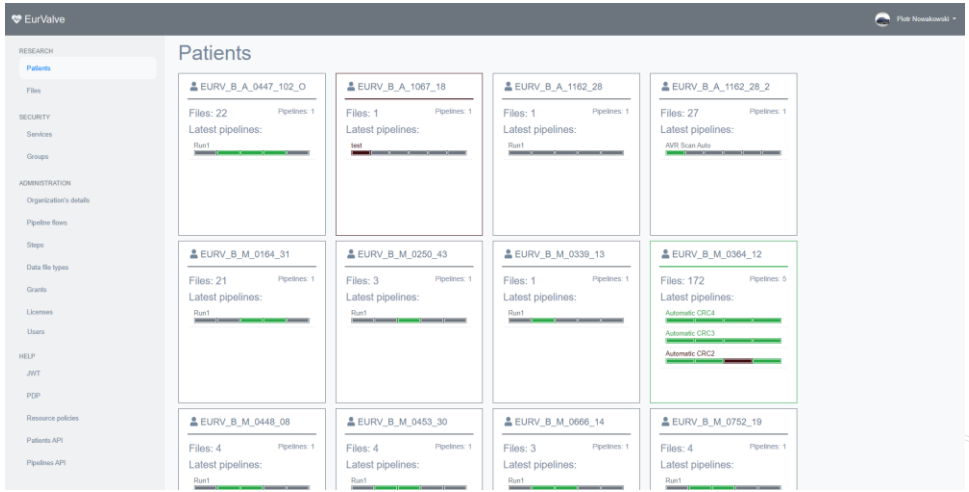
Processing scientific simulations – a conceptual framework

Five main elements required when processing patient cases:

1. HPC infrastructure -> Prometheus cluster
2. Running jobs on Prometheus via RESTful API -> Rimrock
3. Managing data stored on Prometheus via RESTful API -> PLGData
4. Model repository and versioning -> GitLab
5. Managing model execution on patient data -> MEE



Running simulations on integrated patient records



Each computational task is executed in the context of a specific case (e.g. a specific patient) and assumes the form of a pipeline

- A pipeline consists of one or more computational steps, each of which can be assigned required input and output files
- Steps are executed when their required input files are present in the HPC infrastructure – this enables sequential execution of steps; however, many steps may also be executed at the same time if they are capable of running in parallel.
- Each step corresponds to an executable which is stored and versioned in a GitLab repository – this enables repeatability and provenance tracking of output data
- Dedicated step templates are provided for stage-in and stage-out of input and output data for models which entail Big Data analyses.
- The environment provides graphical visualization of the execution status, and also enables platform users to define custom steps and custom pipelines.

Security

Sano uses mainly external infrastructure:

- *Central authentication: e.g. for communication and NextCloud storage*
- *Code and developer communication in private GitHub repositories*

Several security related processes have been implemented:

- *Several data security related SOPs in place*
- *Consulting agreement with an external data protection expert and appointment of a data protection officer (DPO)*

Involvement in Standards

Sano (or third party manufacturers) need to comply with EU **(CE marking)** *and other regulations to market clinical decision software systems (CDSS).*

- **Certification:** *MDR (Medical Device Regulation) 2017/745:*
  - *Applicable ISO standards: ISO 14971 (risk management), IEC 62304 (software lifecycle) and IEC 62366 (usability) in medical devices*
  - *Quality management system: ISO 13485, certified by a notified body, e.g. PCBC (Poland)*
- **Registration:** *National registries, e.g. URPL (Poland), EUDAMED database*
- *Additional regulations for international markets, e.g. HIPAA (US)*

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