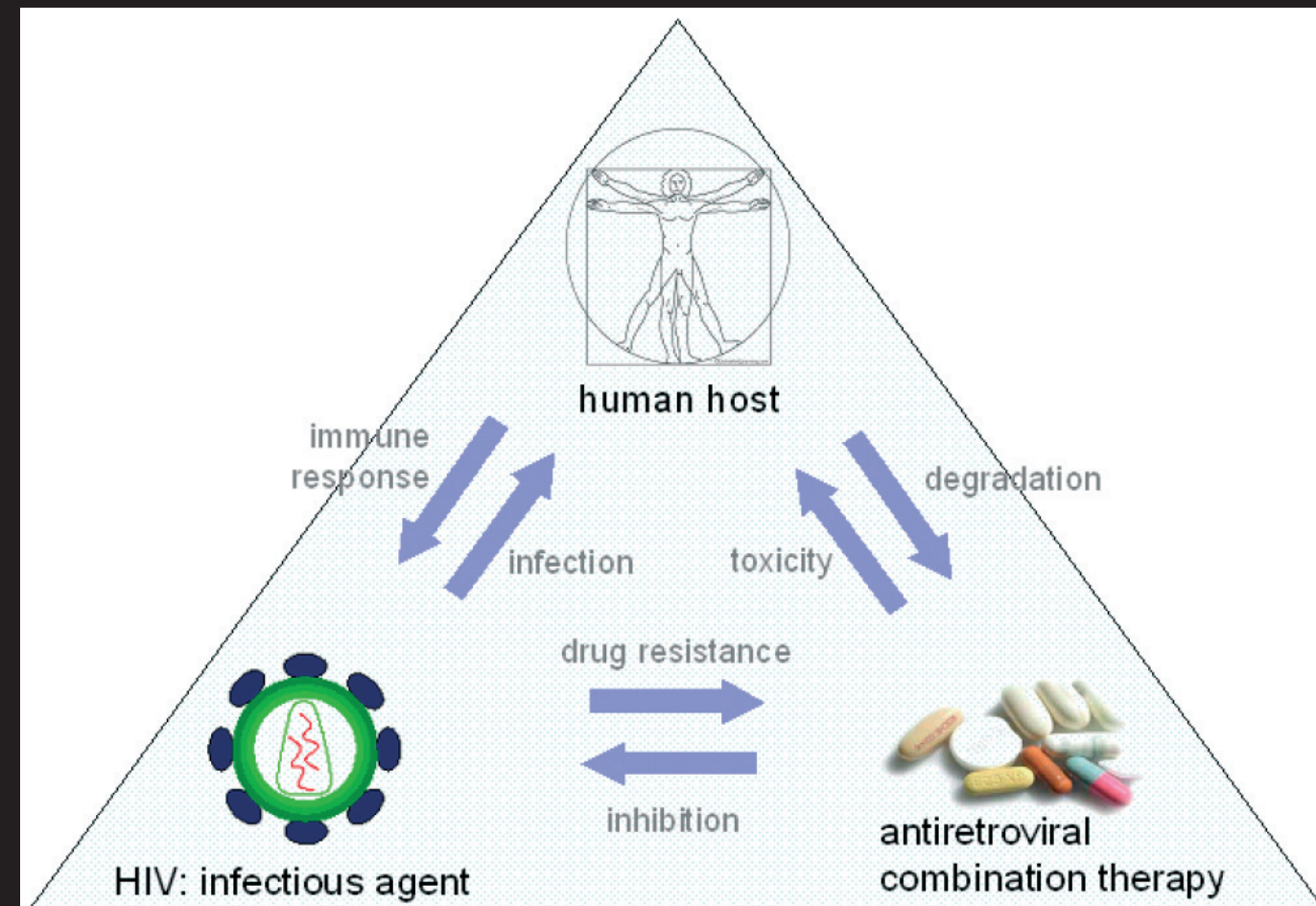# Towards Innovative Healthcare Grid Solutions:
ViroLab – A Virtual Laboratory for Infectious Diseases

Mission of ViroLab

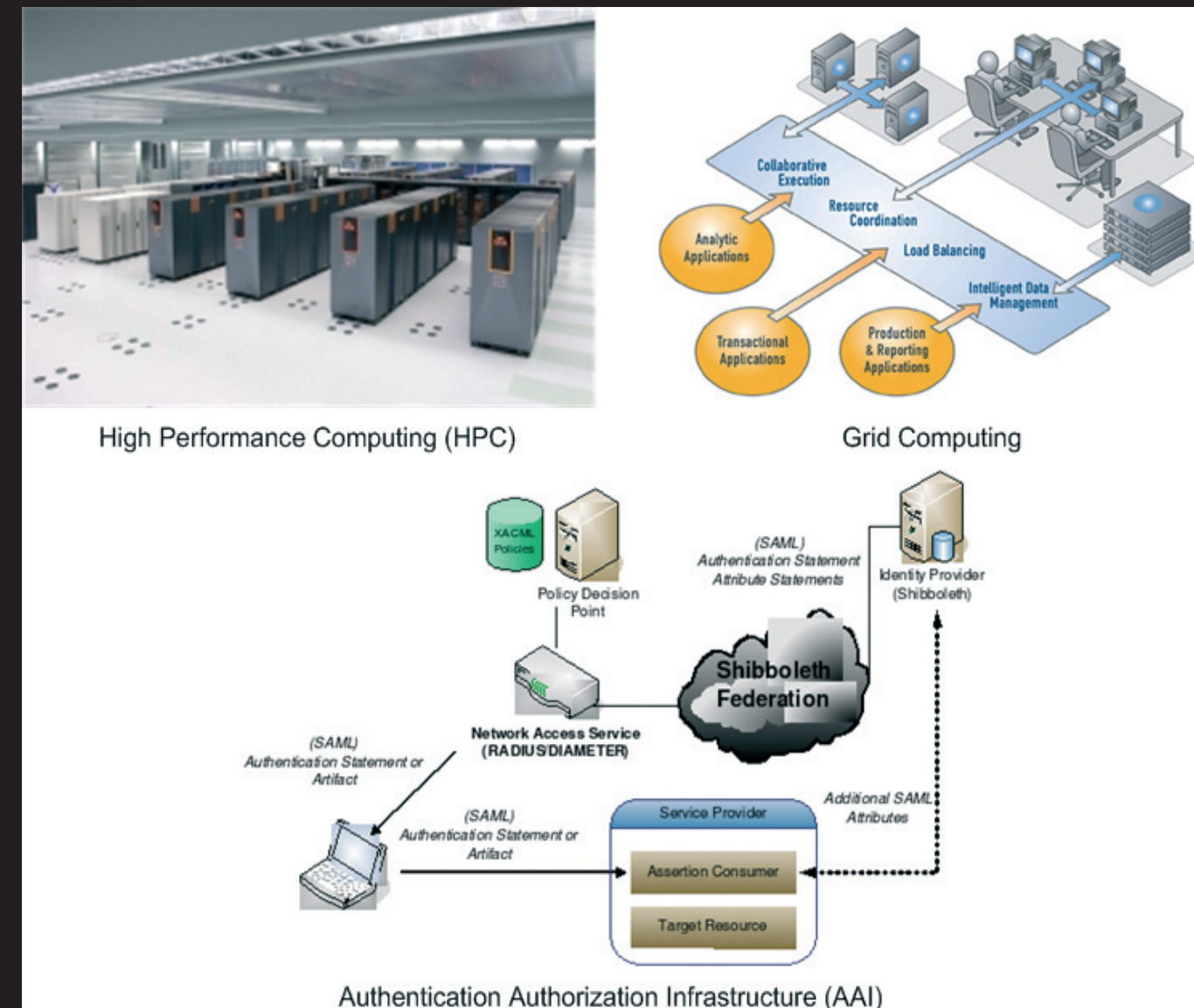|	HIV-infected adults and children	HIV prevalence among adults (%)	New infections per day	Daily deaths from AIDS
Subsaharian Africa	25,000,800	7.2	8,700	6,500
South and Southeast Asia	7,400,000	0.7	2,700	1,300
Eastern Europe and Central Asia	1,600,000	0.9	740	170
Latin America	1,800,000	0.6	550	180
East Asia	870,000	0.1	380	110
North Africa and Middle East	510,000	0.2	180	160
North America	1,200,000	0.7	120	50
Carribean	300,000	1.6	80	70
Western and Central Europe	720,000	0.3	60	30
Australia, New Zealand and Pacific Region	74,000	0.5	20	10
Total	40,300,000	1.1	13,530	8,580

The AIDS Epidemic

- AIDS is the fastest growing infectious disease on earth
- HIV treatment made significant progress over the past years
- Several antiretroviral drugs available which reduced mortality drastically
- Health professionals are currently fighting against new phenomenon of modern medicine: Drug Resistance
- More and more people are living with drug resistant viruses and even a small proportion of patients die because there are no drugs to inhibit their viruses

→ ViroLab – an EU funded STREP within 6th Framework Programme in the area of integrated biomedical information for better health – as a prototype for a virtual laboratory for infectious diseases that facilitates medical knowledge discovery and decision support for HIV drug resistance.

Approach

The Complexity of HIV Treatment

- Complex interplay in HIV treatment requires an interdisciplinary collaboration of multiple sciences
- One needs all scales, all disciplines and all data
- From molecule to man to mankind
- Integration of methodologies from different domains like obtaining information from literature, simulating drug-protein complexes and immuse responses, analyzing temporal data and population trends, and finally deriving rules for decision support

→ Provide user-friendly collaborative working environment available for clinicians and researcher distributed over Europe, which allows

  1.) Usage of well-defined rule sets in order to correctly predict virological and immunological repsonse for all antiretroviral drugs

  2.) Planning of experimental workflows for computing and analyzing genotypic resistance using specific interpretation tools.

Technological Requirements

Technologies addressed by ViroLab

- High Performance Computing (HPC): Mesoscopic simulation and analysis of biological processes demand strong computational power due to their complexity and immense varity of chemical compositions
- Grid Computing:
  - Distributed Data Management:
    Federation and integration of heterogeneous and distributed data resources should be transparent to and hidden from the users by creating virtualization services that combine data disclosure and data fusion capabilities in a simple but at the same time efficient way
  - Virtual Organization (VO):
    Building a VO for secure exchange of confidential and private information (patient data) between several organizations using state-of-the-art Grid technologies, this VO should also form the „glue" for all ViroLab Virtual Laboratory components.
- Authentication Authorization Infrastructure (AAI):
  Strong mechanisms for user identification as well as service / resource authorization need to be set up for ViroLab in order to prevent the abuse of sensible data.

German e-Science Conference 2007
May 2nd – 4th, 2007
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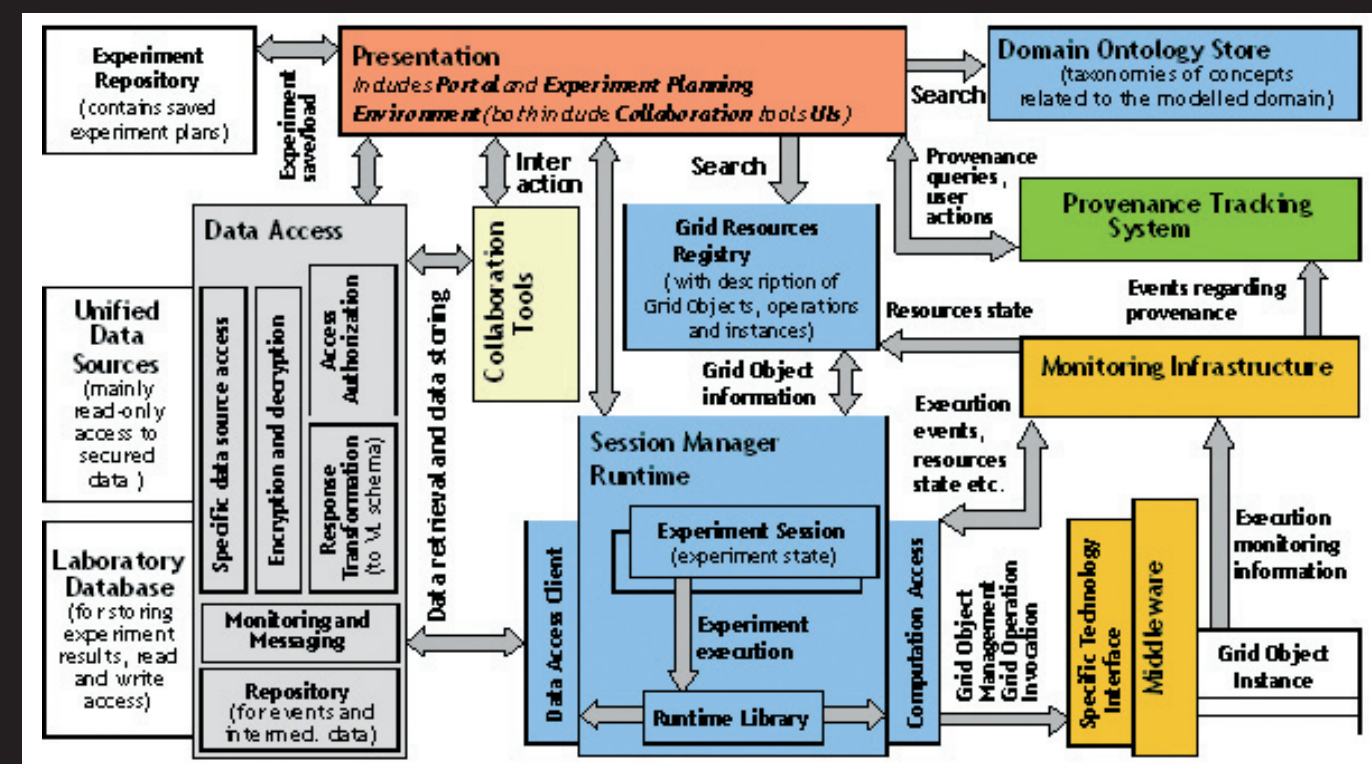
Authors:

Assel Matthias (assel@hlrs.de)

Krammer Bettina (krammer@hlrs.de)

HLRS – High Performance Computing Center Stuttgart
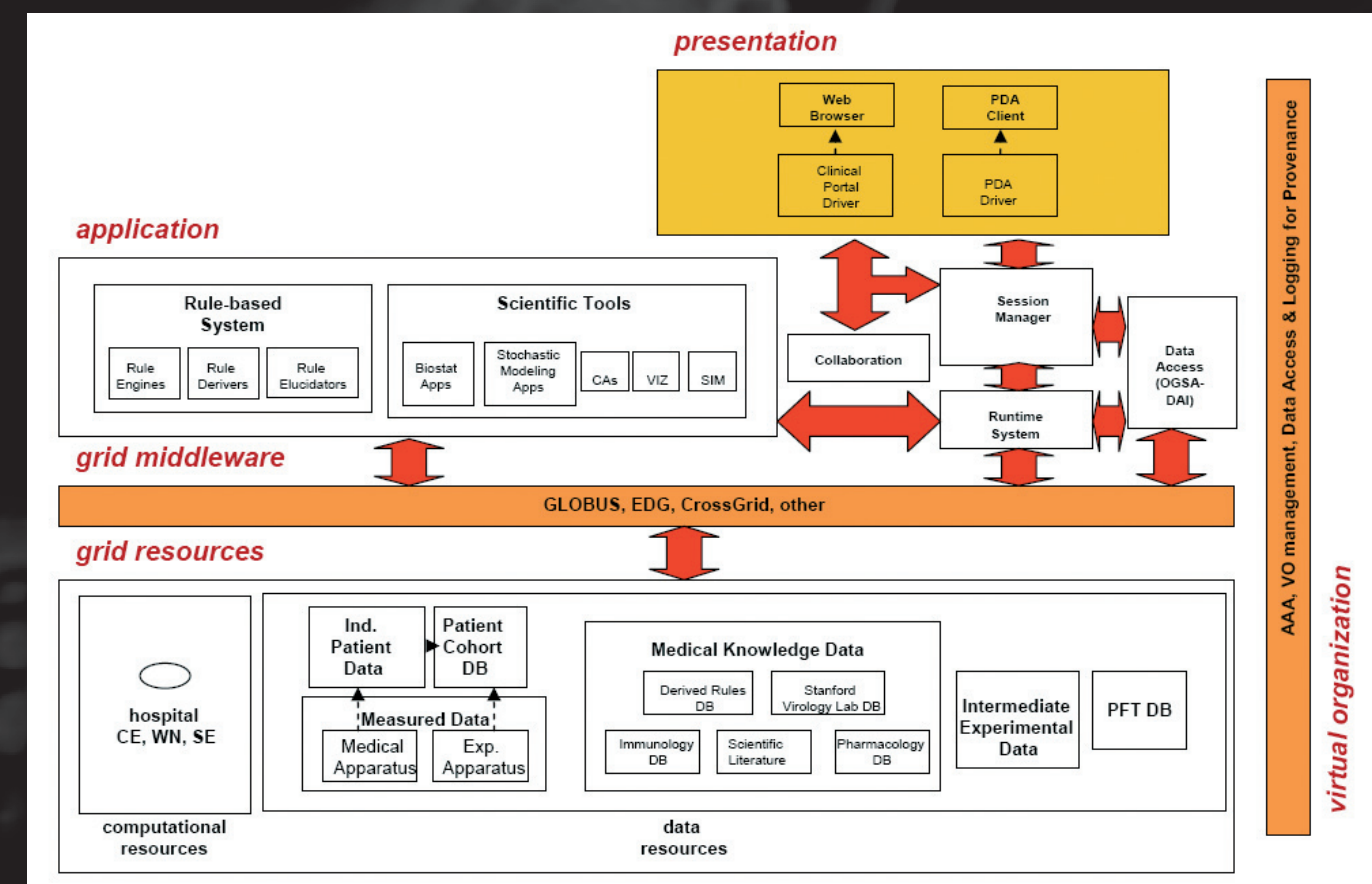
Nobelstr. 19, 70569 Stuttgart, Germany

Partner

- University College London, United Kingdom
- Gridwisetech, Poland
- ACK Cyfronet AGH, Poland
- Eotvos Lorand University, Hungary
- Catholic University of Leuven, Belgium
- IRSICAIXA Foundation, Spain
- Catholic University of Rome, Italy
- University of Brescia, Italy
- University of Stuttgart, HLRS, Germany
- University of Amsterdam, The Netherlands
- University Medical Center Utrecht, The Netherlands
- Virology Education, The Netherlands

The ViroLab Virtual Laboratory

General Laboratory Architecture

The Core Components of ViroLab

- Virtual laboratory to be used by medical doctors to review previous results and rankings and / or scientists to conduct new experiments starting from pre-defined process flow templates
- Topmost part is devoted as *Presentation Layer* through which the user interacts with the system
- Two main user interfaces including collaboration tools to be supported:
  1.) *ViroLab Portal* defining the entry point for scientists and medical doctors
  2.) *Experimental Planning Environment* (EPE) provided for experiment developers
- The *Domain Ontology Store* and the *Grid Resources Registry* support developers to find proper computational and data resources for their planned experiments
- All data access operations are coordinated by the *Data Access* module which is directly linked with the *Presentation* and the *Runtime system*
- *Monitoring Infrastructure* responsible for acquiring, storing and providing interesting events in the form of notifications or responses to queries
- *Provenance Tracking System* stores all information relevant from the point of view of data (results) and publishes that information for interesting parties

Virtual Organization Architecture

The ViroLab Virtual Laboratory from the Grid (VO) Perspective

- VO concept mainly used for access control of requested resources
- Architecture divided into three main layers:
  1.) *Presentation*: Front-end for ViroLab users
  2.) *Security Infrastructure*: AAI and mechanisms for data encryption
  3.) *Middleware Stack*: Access to different grid middleware solutions (GT4, EGEE)
- Presentation layer contains all interfaces and is responsible for user authentication by interacting with the security layer
  - AAI using Shibboleth approach
  - Grid-Security Infrastructure (GSI) for secure communication
  - Authorization decision always taken by the service / data provider based on user's attributes due to confidentiality of data
- Goal of middleware subsystem is to reuse existing grid middleware and infrastructure that are accessible to the partners without developing specific solutions from scratch
- Main focus on resource management (access to computation) and information management (access to monitoring)

Summary

- Design and development of medical software solutions constitute one of the challenging fields in computer sciences

- ViroLab accepts this challenge in order to support doctors and researchers in addressing the problem of HIV drug resistance

- Integration of biomedical data resources into a collaborative working environment as a particular and challenging field in Grid Computing

- Security aspects of utmost significance due to confidentiality of shared information and strong legal and ethical issues for medical data

→ ViroLab to encourage people to focus their research on complex medical interplay using Grid infrastructure

References:

Deeks S. Treatment of antiretroviral.drug-resistant, HIV-1 infection. Lancer 2003; 362(9400):2002-2011.

Jaggy C., von Overbeck J., Ledergerber B., Schwarz C., Egger M., Rickenbach M. et al. Mortality in the Swiss HIV Cohort Study (SHCS) and the Swiss general population. Lancet 2003; 362(9387):877.878.

Nijhuis M., Deeks S., Boucher C. Implications of antiretroviral resistance on viral fitness. Curr Opin Infect Dis 2001; 14(1):23-28

ViroLab – EU IST Project (IST-027446). http://www.virolab.org

Sloot P., Boucher C., Bubak M., Hoekstra A., Plaszczak P., Posthumus A., van de Vijver D., Wesner S. and Tirado-Ramos A. VIROLAB – A Virtual Laboratory for Decision Support in Viral Diseases Treatment. Cracow Grid Workshop 2005, Cracow, Poland, November 2005.

Assel M., Krammer B., Loehden A. Management and Access of Biomedical Data in a Grid Environment. Cracow Grid Workshop 2006, Cracow, Poland, October 2006.

Barton T., Basney J., Freeman T., Scavo T., Siebenlist F., Welch V., Ananthakrishnan R., Baker B., Goode M., Keahey K. Identity Federation and Attribute-based Authorization through the Globus Toolkit, Shibboleth, GridShib, and MyProxy. Proceedings of 5th Annual PKI R\,&D Workshop. March 2006.

Bubak M., Gubala T., Malawski M., Kasztelnik M., Bartynski T., Nowakowski P. Virtual Laboratory in ViroLab. Cracow Grid Workshop 2006, Cracow, Poland, October 2006.

Filipovic B., Straub T. Grid Security Infrastructure – Ein Ueberblick. 20. DFN-Jahrestagung. Heilbronn, Germany, June 2006.