# Computational Biomedicine: A Challenge for the 21st Century

**Peter V Coveney**

Centre for Computational Science

University College London

p.v.coveney@ucl.ac.uk

# Overview

- The UCL Centre for Computational Science
- Computational Biomedicine Case Studies
- Medical Data Storage and Security issues
- The Virtual Physiological Human initiative
- EU e-Infrastructure Projects for Biomedical Data Management & Processing
- Conclusions

# Centre for Computational Science:

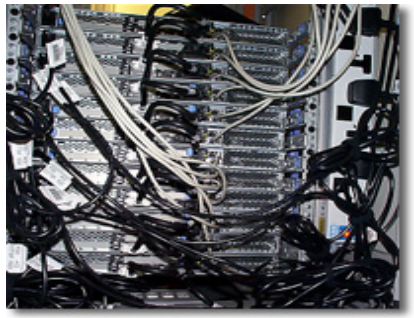
## "Advancing science through computers"

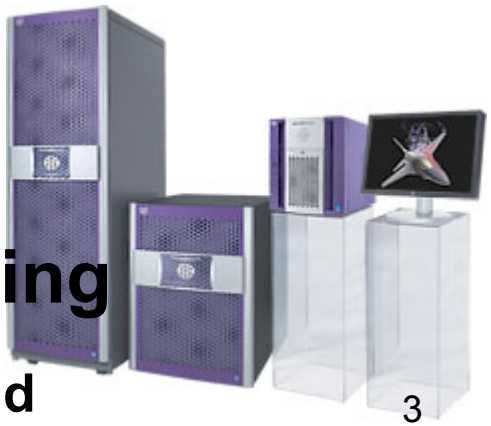
**Computation/computational science/computer science is central to modern science.**

**Computational infrastructure both empowers and circumscribes much of what is scientifically achievable.**

**serial** → **parallel** → **grid computing** → **cloud computing**

P. V. Coveney and R. R. Highfield, *Frontiers of Complexity* (1995)





**Internet** → **Web** → **Grid/Cloud**

## *Advancing science through computers*

- *Computational Science*
- *Algorithms, code development & implementation*
- *High performance, data-intensive & distributed computing*
- *Visualisation & computational steering*
- *Condensed matter physics & chemistry, materials & life sciences*
- *Translational medicine, e-Health & VPH – "data deluge"*

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# Patient-specific medicine

- ‘Personalised medicine’ - use the patient’s genotype/phenotype to better manage disease or predisposition towards a disease
- Tailoring of medical treatments based on the characteristics of an individual patient

## *Why use patient-specific approaches?*

- Treatments can be assessed for their effectiveness with respect to the patient before being administered, saving the potential expense and trauma of multiple/ineffective treatments

## *Patient-specific medical-simulation*

- Use of genotypic and/or phenotypic simulation to customise treatments for each particular patient -- computational modelling can be used to predict the outcome of courses of treatment and/or surgery

# Case study I : Grid Enabled Neurosurgical Imaging Using Simulation

**The GENIUS project aims** to model large scale patient specific cerebral blood flow in clinically relevant time frames

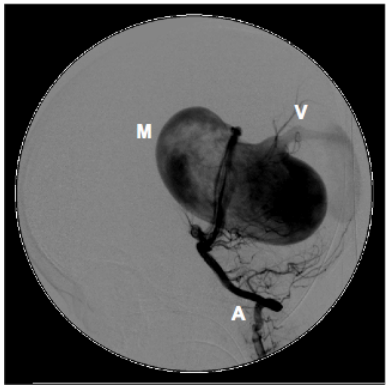
**Original objectives**:

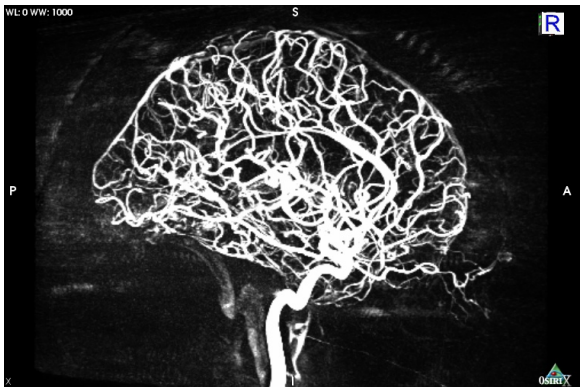
- To study cerebral blood flow using patient-specific image-based models.
- To provide insights into the cerebral blood flow & anomalies.
- To develop tools and policies by means of which users can better exploit the ability to reserve and co-reserve HPC resources.
- To develop interfaces which permit users to easily deploy and monitor simulations across multiple computational resources.
- To visualize and steer the results of distributed simulations in real time

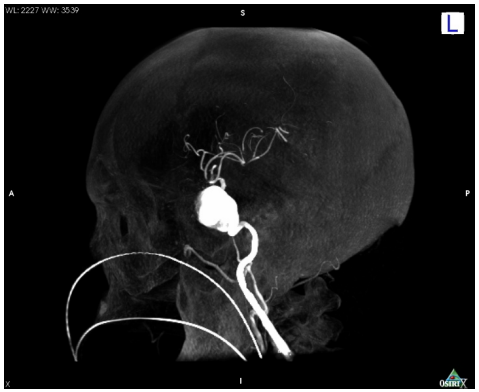
# Clinical Supercomputing

## *Diagnosis and decision support in surgery*

- Provide simulation support from *within the operating theatre for* neuroradiologists
- ***Provide new information to surgeons for patient management and therapy***:
  1. Diagnosis and risk assessment
  2. Predictive simulation in therapy
- Provide patient-specific information which can help plan embolisation of arterio-venous malformations, coiling of aneurysms, etc.



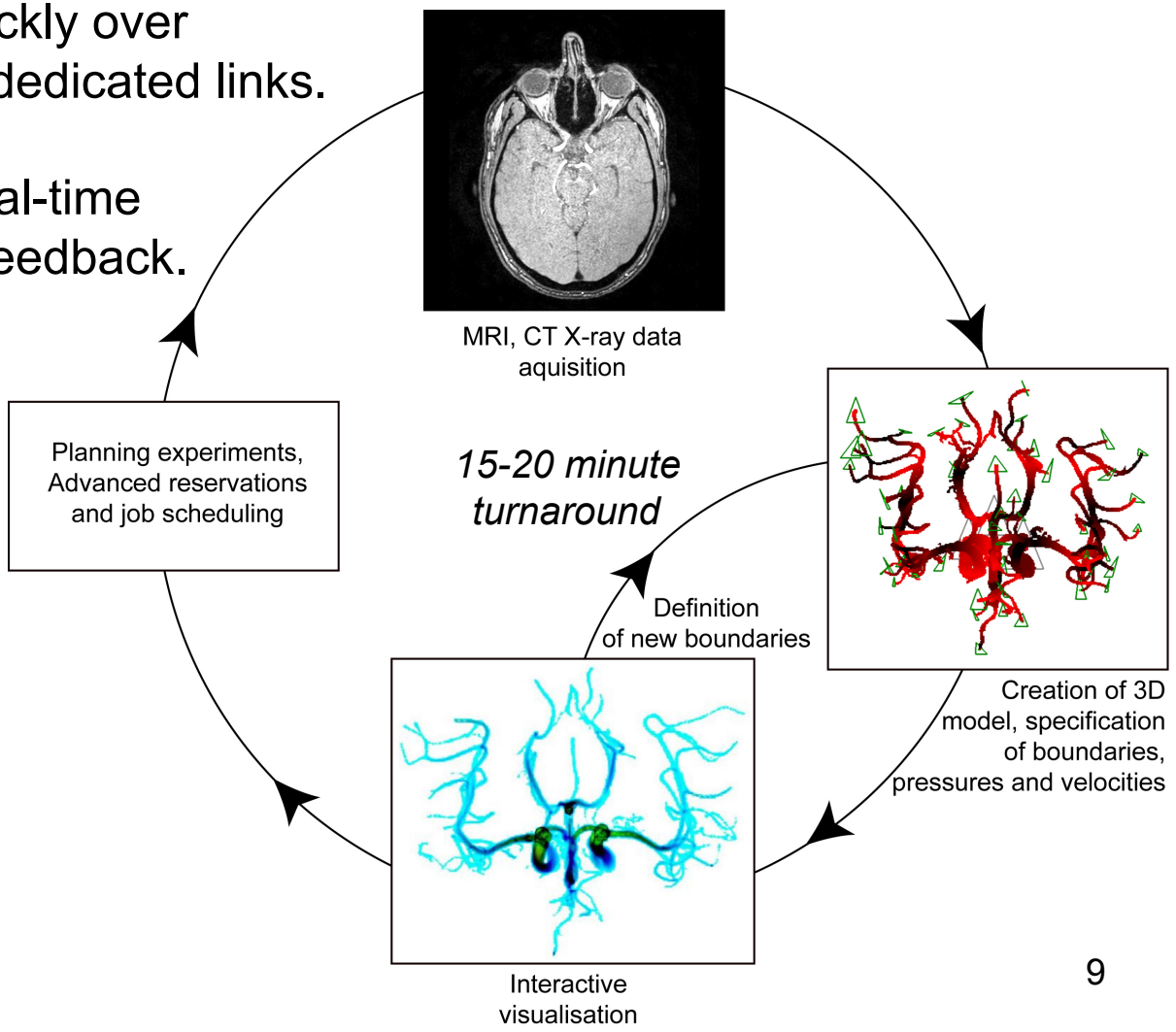



# GENIUS clinical work flow

Book computing resources in advance or have a system by which simulations can be run urgently.

Shift imaging data around quickly over high-bandwidth low-latency dedicated links.

Interactive simulations and real-time visualisation for immediate feedback.



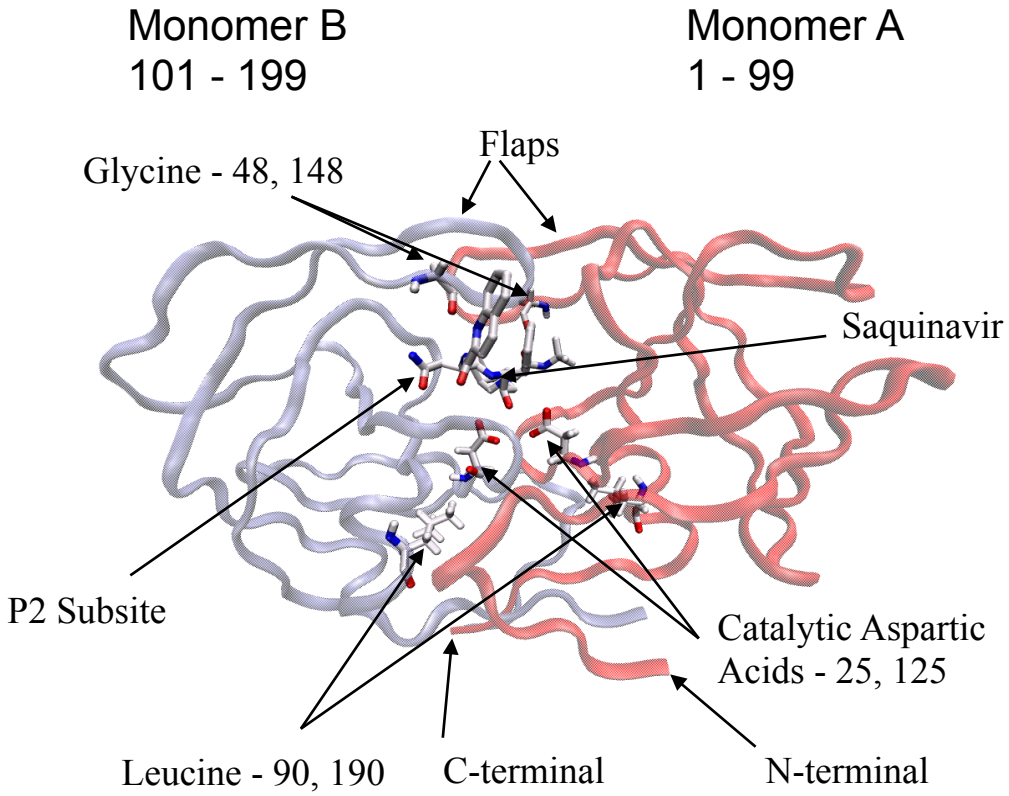
# Case study II : Patient-specific HIV drug therapy

## HIV-1 Protease is a common target for HIV drug therapy

- Enzyme of HIV responsible for protein maturation
- Target for Anti-retroviral Inhibitors
- Example of Structure Assisted Drug Design
- 9 FDA inhibitors of HIV-1 protease

**So what's the problem?**

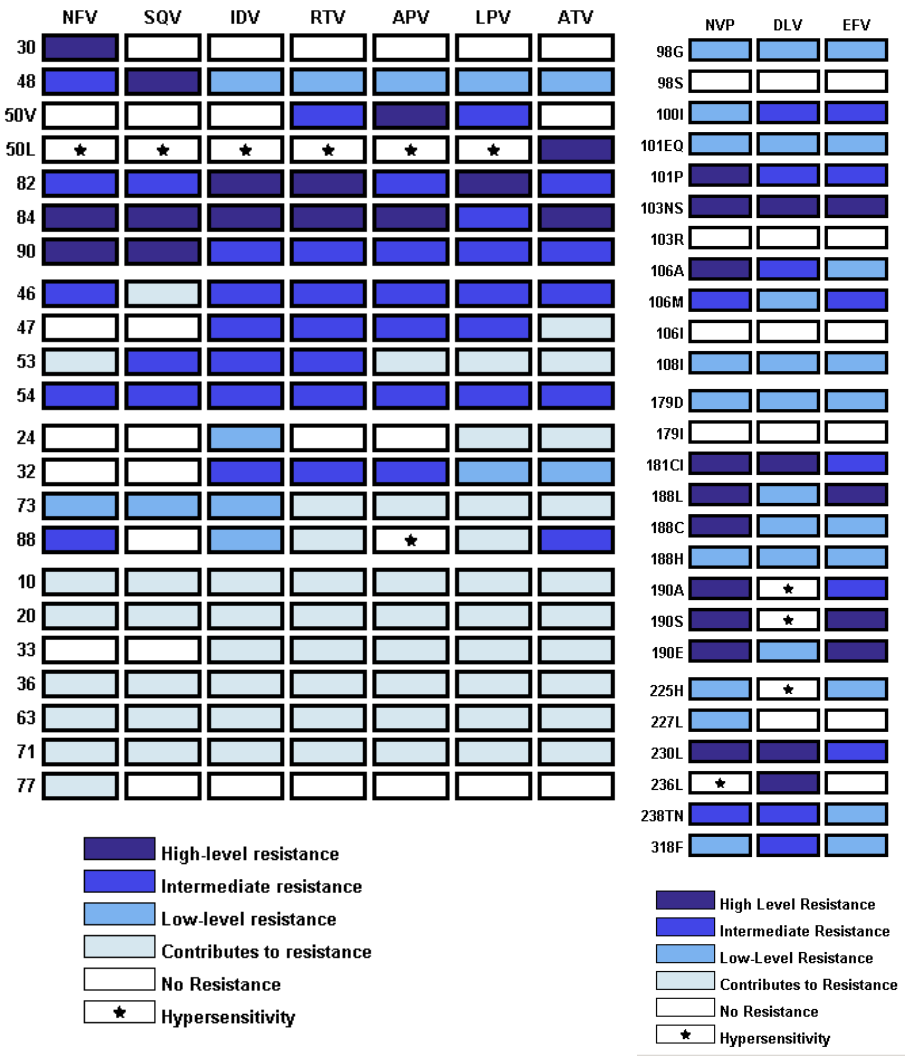
- Emergence of drug resistant mutations in protease
- Render drug ineffective
- Drug resistant mutants have emerged for all FDA inhibitors




**EU FP6 ViroLab project, EU FP7 CHAIN & VPH-SHARE projects**

P. M. A Sloot, P. V. Coveney et. al., "HIV decision support: from molecule to man", Phil. Trans. R. Soc. A., **367**, (1898), 2691-2703, (2009).

# Clinical decision support

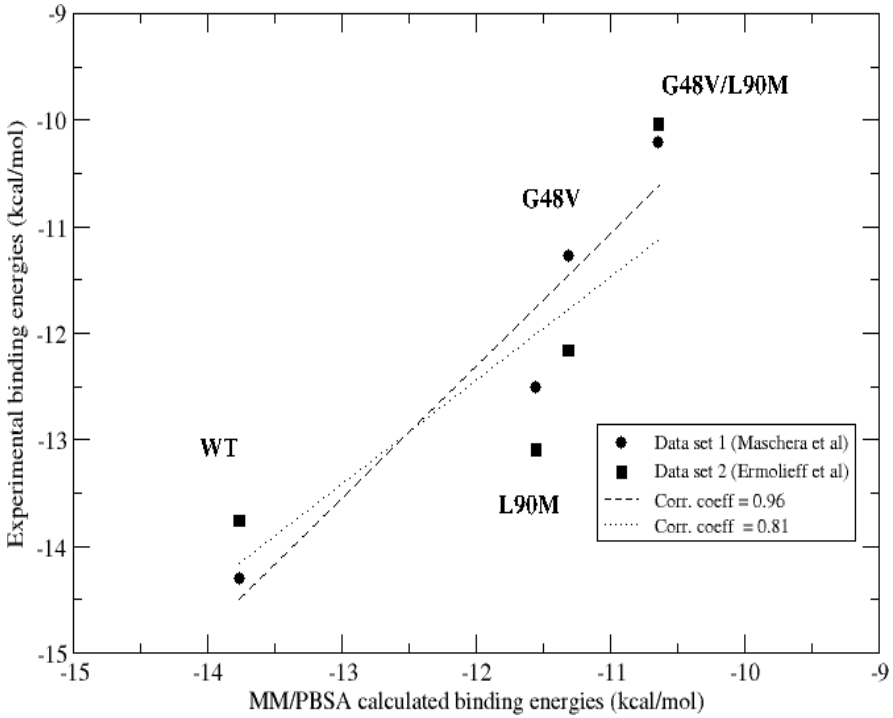



- Too many mutations to interpret by a clinician
- Support software is used to interpret genotypic assays from patients
- Uses both *in vivo* and *in vitro data*
- Is dependent on
  - Size and accuracy of *in vivo* clinical data set
  - Amount of *in vitro* phenotypic information available - e.g. binding affinity data

# Binding of saquinavir to wildtype and resistant HIV-1 proteases L90M and G48V/L90M

**Thermodynamic decomposition**

- explains the distortions in enthalpy/ entropy balance caused by the L90M and G48V mutations
- absolute drug binding energies are in **excellent agreement** (1 – 1.5kcal/mol) with experimental values
- Data-driven, data intensive, high performance computing challenge

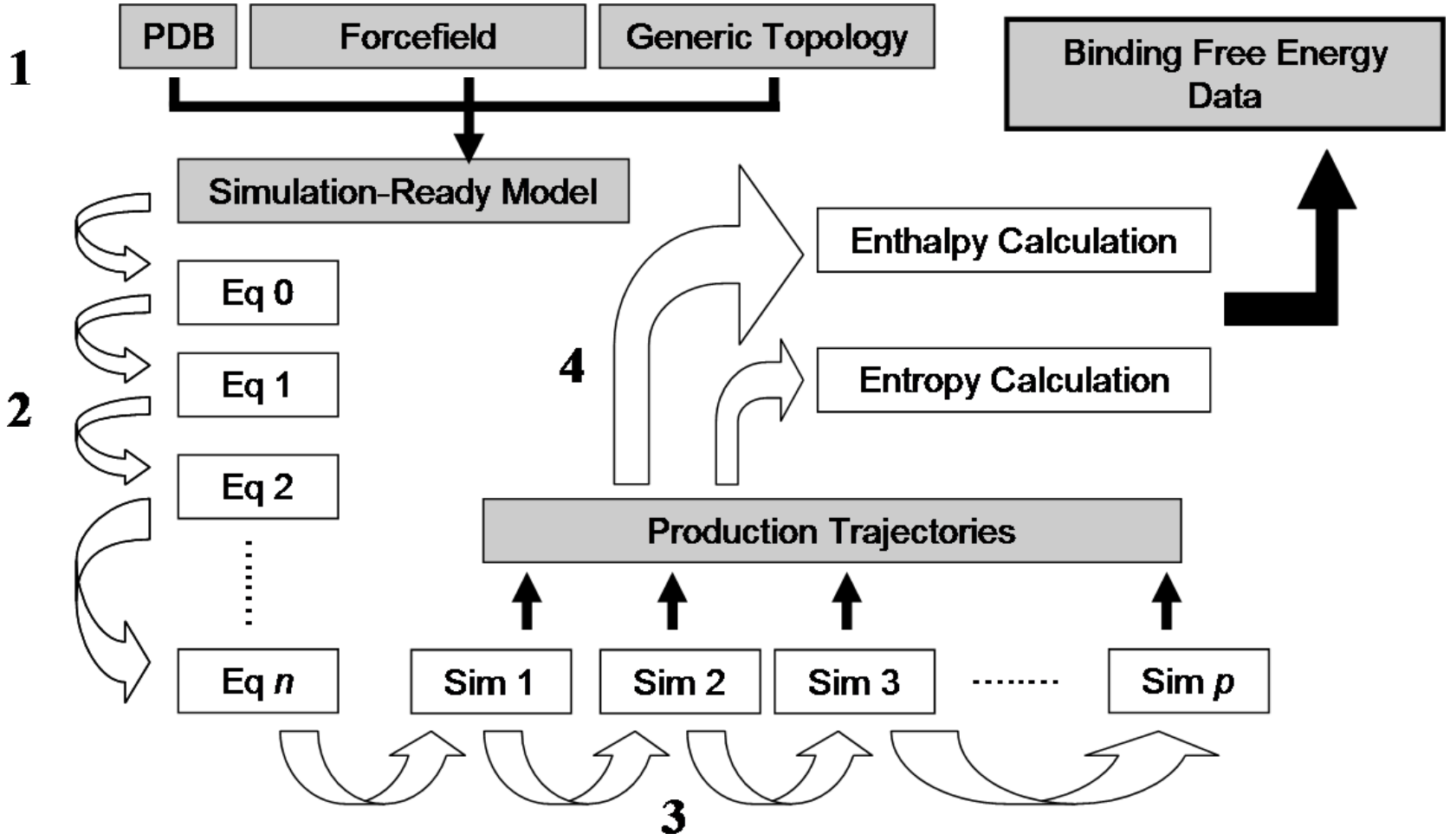



**Applications used include: NAMD, CHARMM, AMBER…**

**Rapid and accurate prediction of binding free energies for saquinavir-bound HIV-1 proteases.**
Stoica I, Sadiq SK, Coveney PV. J Am Chem Soc. 2008;130(8):2639-48.

# Binding affinity – data intensive workflow

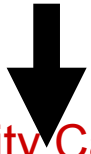
**Molecular Mechanics Poisson-Boltzmann Surface Area (MMPBSA) & Entropy Calculation**




**Applications used include: NAMD, CHARMM, AMBER…**

# Automation of binding affinity calculation

- Aim is to provide tools that allow simulations to be used in a clinical context
- Require large number of simulations to be constructed and run automatically
  - To investigate generalisation
  - Automation is critical for clinical use
- Turn-around time scale of around a week is required
- Trade off between accuracy and simulation turn around time



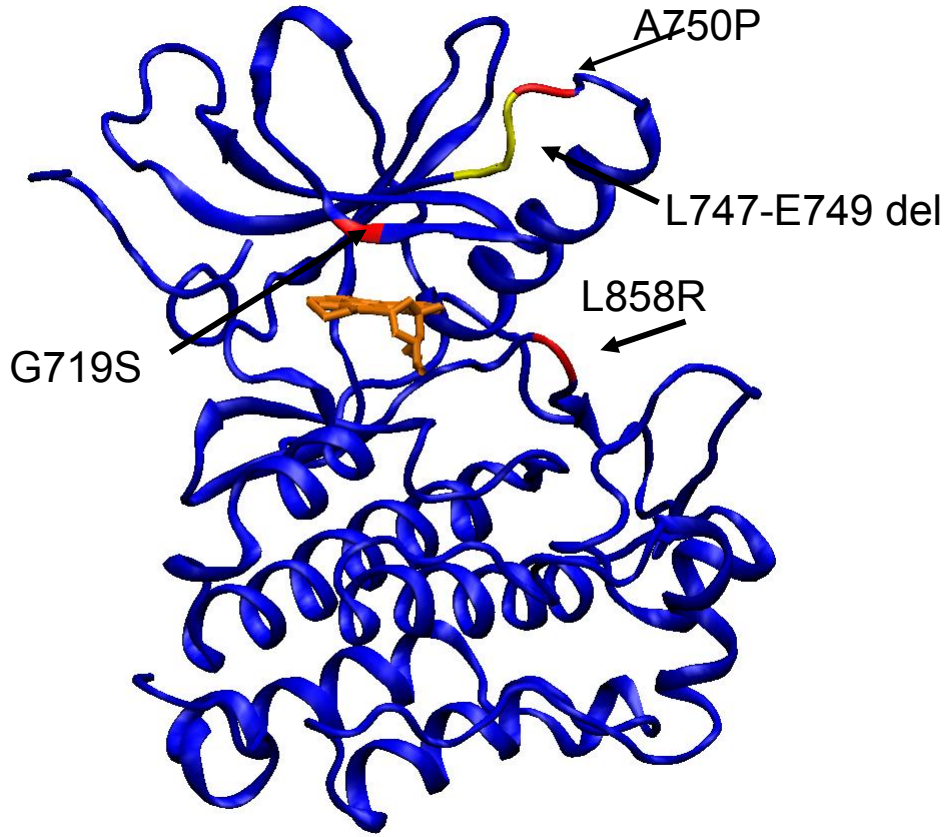
Binding Affinity Calculator (BAC)

*A distributed automated high throughput binding affinity calculator for HIV-1 proteases with relevant drugs*

S. K. Sadiq, D. Wright, S. J. Watson, S. J. Zasada, I. Stoica, Ileana, and P. V. Coveney, "Automated Molecular Simulation-Based Binding Affinity Calculator for Ligand-Bound HIV-1 Proteases", Journal of Chemical Information and Modeling, **48**, (9), 1909-1919, (2008), **DOI: 10.1021/ci8000937**.

# Case study III: Patient specific lung cancer therapies

**EGFR mutations arising in lung cancer**



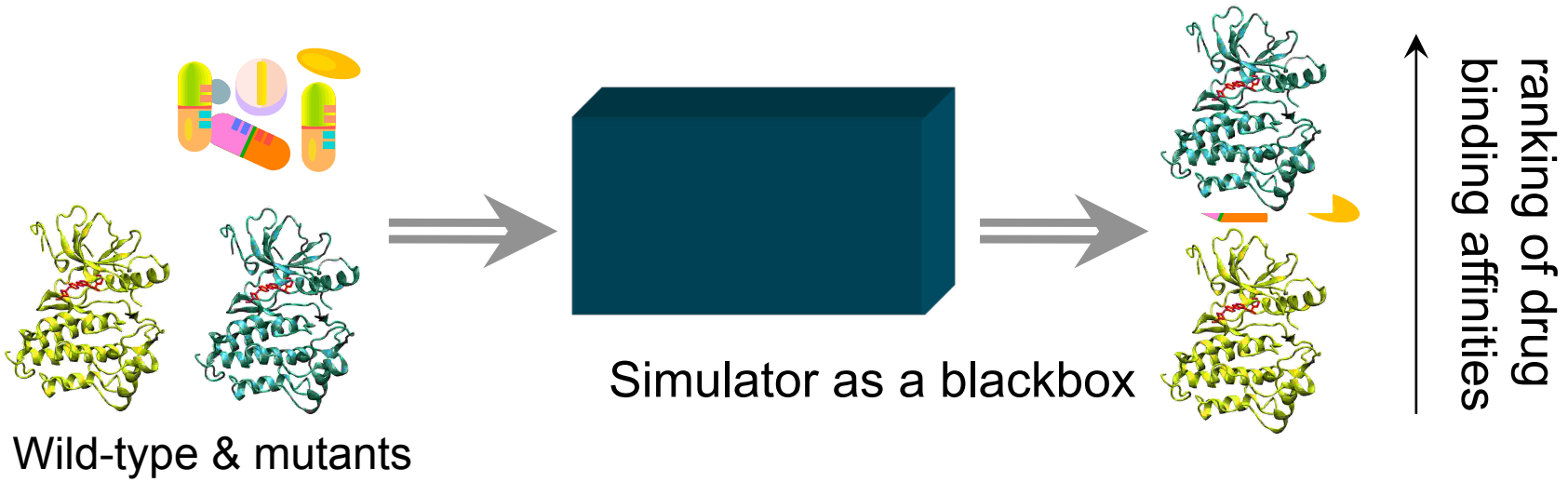

EGFR Tyrosine Kinase Domain

- Over expression of Epidermal Growth Factor Receptor (EGFR) is associated with cancer
- Target for inhibitory drugs
- Important mutations include deletions
- Again binding affinity calculations can be used to determine mutational effects

**Applications used include: NAMD, CHARMM, AMBER, DESMOND, …**

# Biochemical level simulator

Simulator: a decision support software to assist clinicians for cancer treatment, and to reliably predicts patient-specific drug susceptibility




Blackbox: a clinician doesn't need to know anything about the simulator.

**Applications used include: NAMD, CHARMM, AMBER, DESMOND, …**

# Ranking of Binding Affinities

**Gefitinib:**

a) Calculated results are strongly correlated with the experimental values in all cases but L858R mutation.

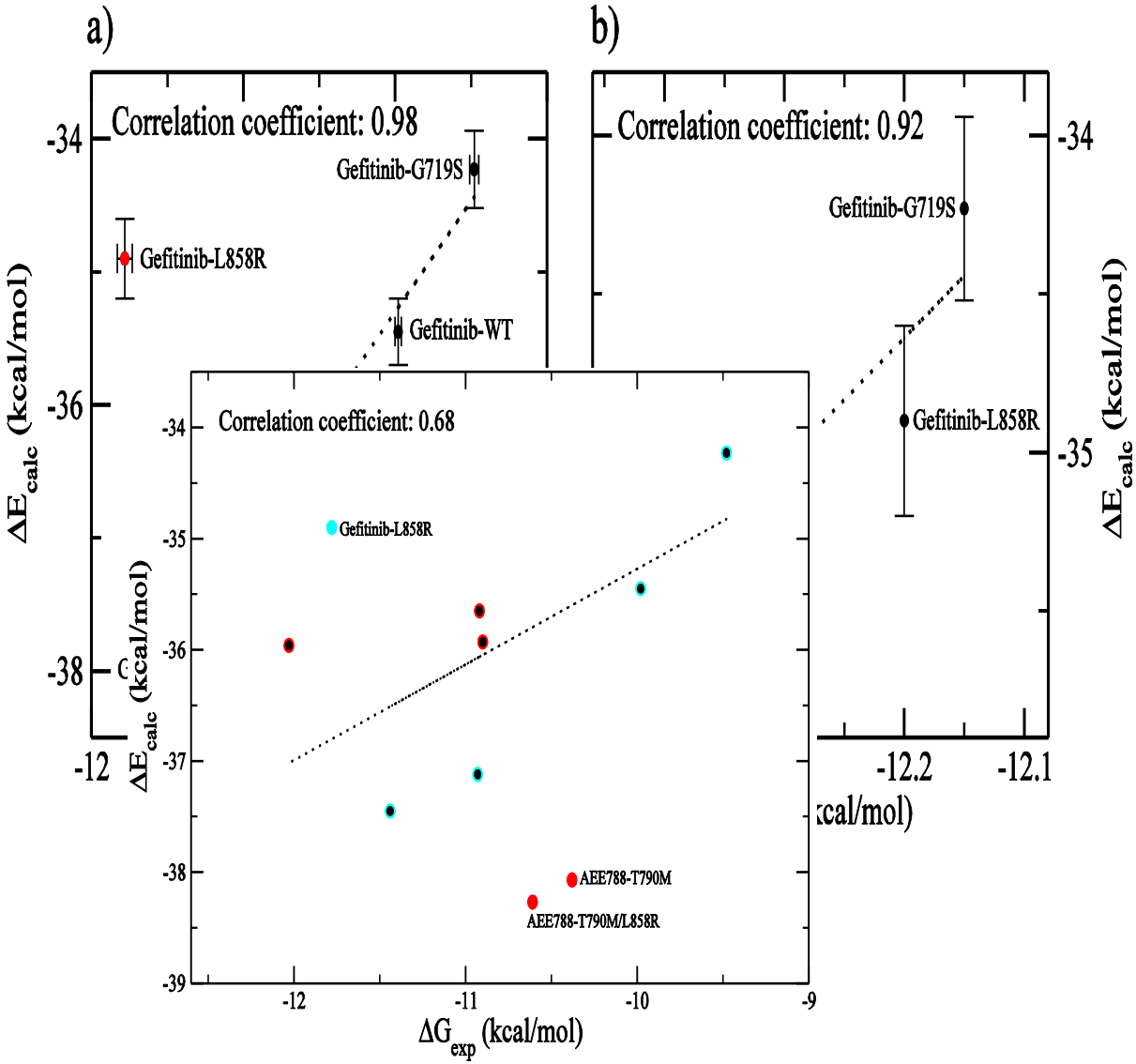
b) The L858R mutation is well behaved when comparing with another experimental date set.

**Gefitinib & AEE788:**

Binding affinity can be ranked for:

– One drug to multiple mutants;

– Efficiency of drugs on a single strain of EGFR.




S. Wan, P. V. Coveney, "Rapid and accurate ranking of binding affinities of epidermal growth factor receptor sequences with selected lung cancer drugs", J. R. Soc. Interface **8**.114-1127, (2011)**, DOI: 10.1021/ci8000937**.

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# Medical Data Storage Issues

- Medical data comprises many types
  - Medical imaging (MRI, CT, etc..) in various formats (e.g. JPEG, DICOM, .xls files, …);
  - Pseudo-anonymised patient information (therapy details, follow up diagnosis, treatments, EHR, etc.)
  - Genomic,  DNA, RNA, protein/proteomics data, etc.
- How to store the above heterogeneous data in one environment?
- How to interface with the various types of data? Understand and use the data (interoperability)
- How to deal with the large size of data resulting from complex simulations, e.g. terabytes and petabytes?
- How to acquire and transfer medical data from resource providers
  - Burn anonymised data on CDs/DVDs and pass them on to researchers vs electronic transfer from provider to data storage directly?
  - **Network connectivity for large simulations and data movements**

# Security /Legal / Ethical issues

Data breach is the unauthorized acquisition, access, use, or disclosure of protected health information.

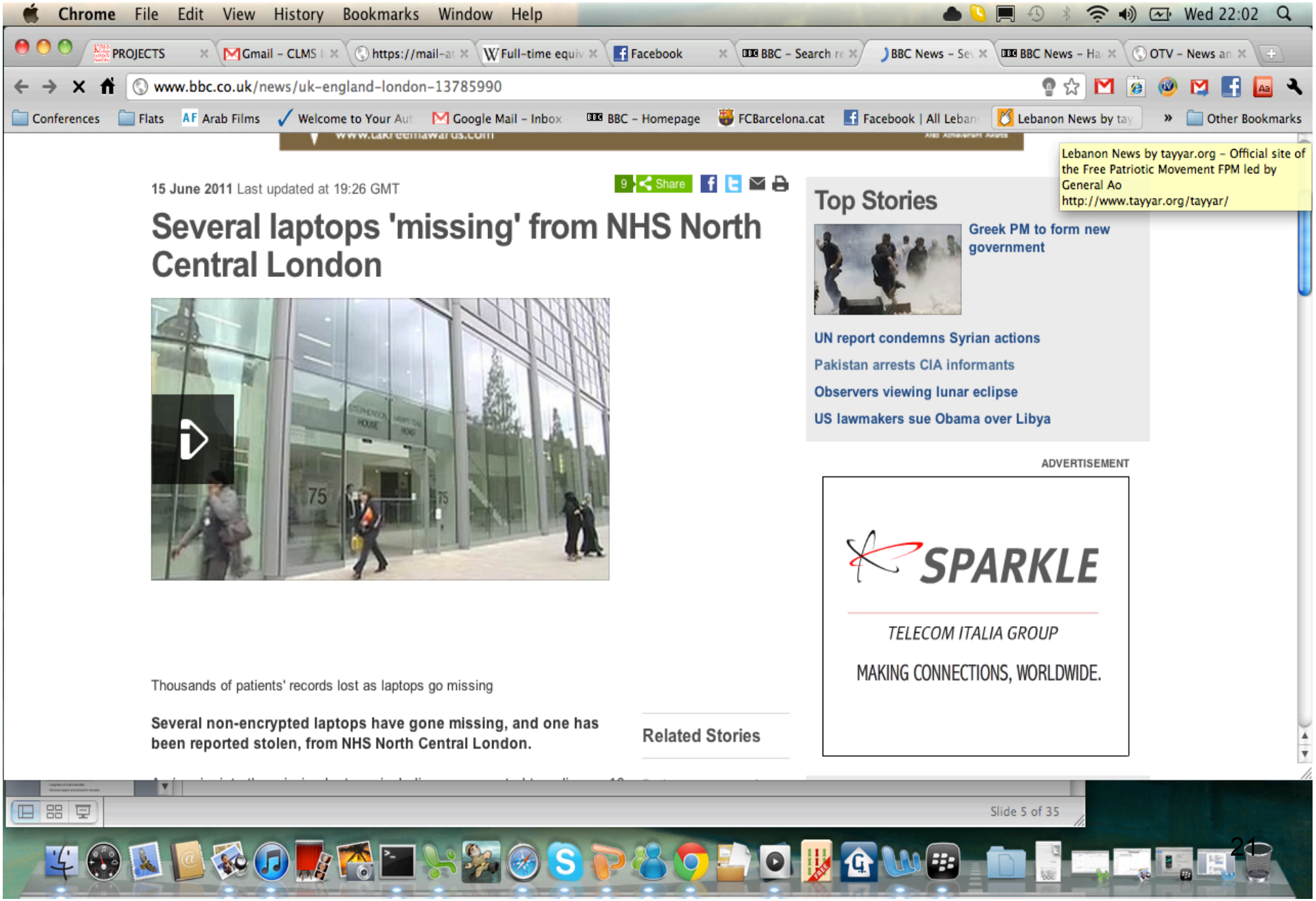
- Complying with legislation:
  - UK Data Protection Act 1998
  - EU Health Directive
  - Patient Confidentiality
- Seamless and secure access to shared data
- Usability of security mechanisms that enable access to shared data

- Patient Consent
- Research Ethics
- Anonymisation
- Incident Management
- Archiving

- Information assurance
  - Who did what and when? ⇒ Authentication, Authorisation, Availability, Integrity and Auditing

- "Centralised" vs "federated" vs "cloud" storage
  - Ownership of data, compliance, what are the applicable laws and regulations governing the data ? Auditing in the cloud?

# Data loss: bad reputation, penalties



# ACD: Usable Security Solution for Accessing Grid Environment and Shared Medical Data

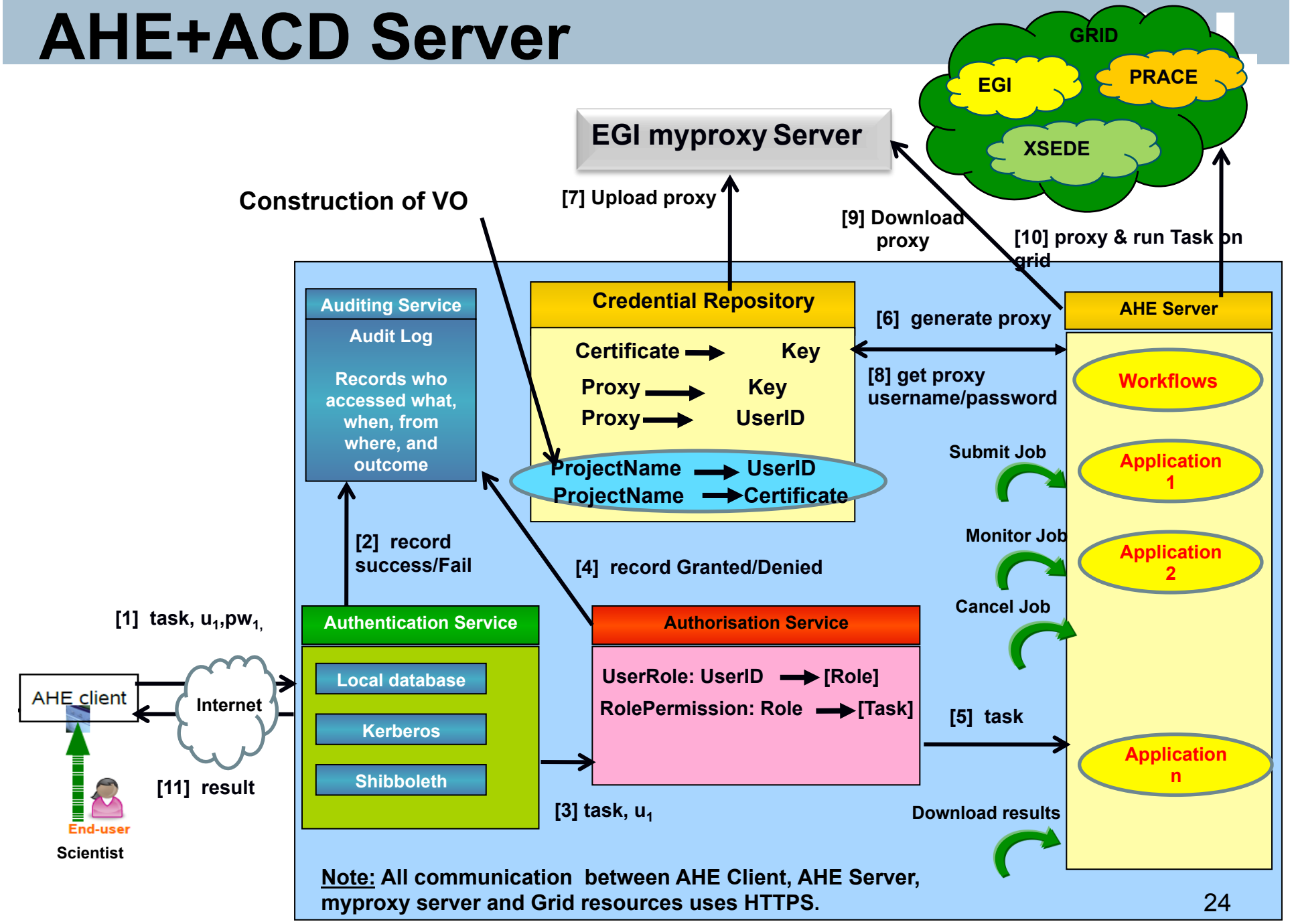
- ***A***udited ***C***redential ***D***elegation (ACD) is a security solution that provides :
  - Alterative authentication methods to certificate based approach. Current prototype supports username/ password mechanism; Shibboleth is underway (expected release Oct 2011).
  - "Hides" the X.509 digital certificate from the end-user; it does not replace it!
  - Authorisation based on parameterised Role Based Access Control
  - Auditing

Haidar A. N., Zasada S. J., Coveney P. V., Abdallah A. E., Beckles B., Jones M. A. S. Audited Credential Delegation: a usable security solution for the virtual physiological human Toolkit. *Interface Focus* **1**, 462–473, 2011.

# ACD status

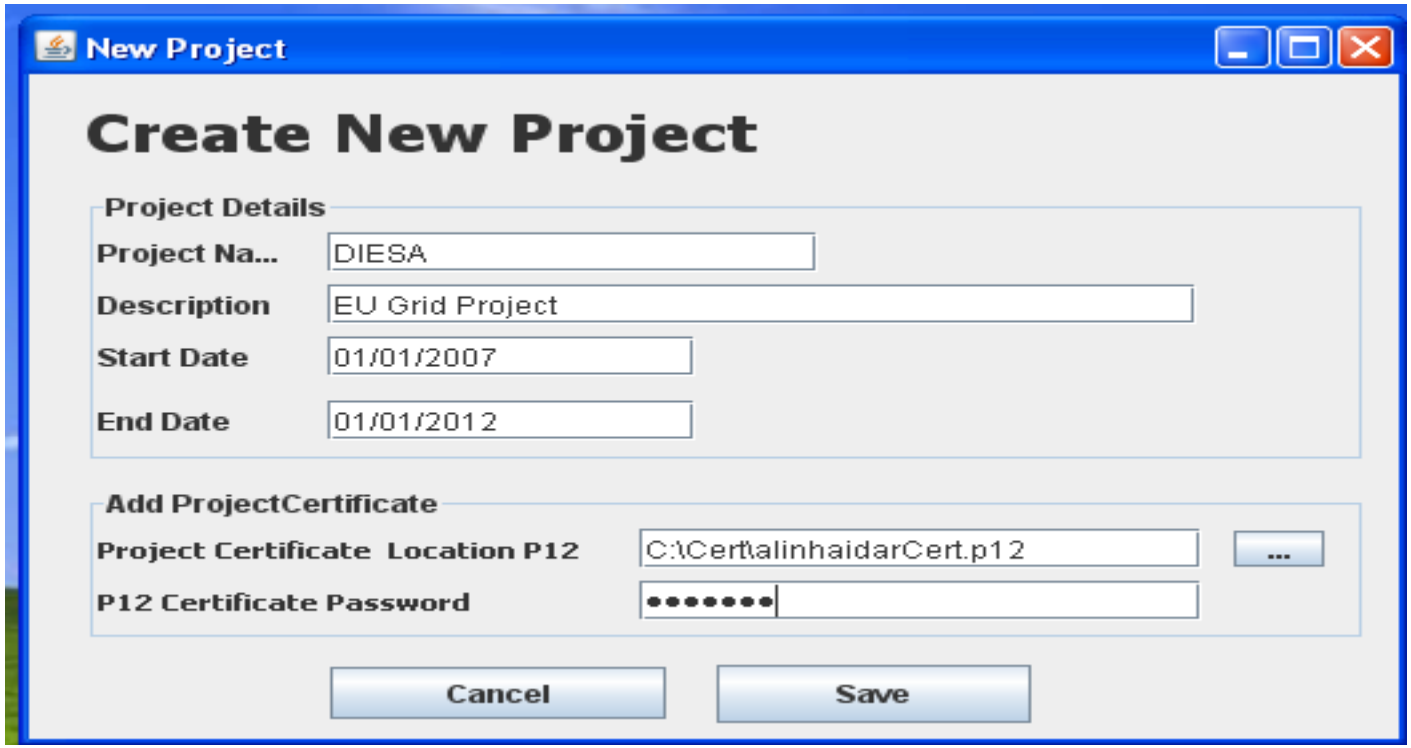
- Currently implemented as a security extension to the Application Hosting Environment (AHE2.0) middleware: http://www.realitygrid.org/AHE/
- Tested and Deployed on XSEDE, EGI and PRACE
- Combination of ACD+AHE is currently on the Science Gateways list of XSEDE
  - https://www.xsede.org/gateways-listing
- Enables construction of VOs that enable scientists to run pre-configured applications/workflows on remote grid resources using familiar credentials such as username-password.

# AHE+ACD Server



# ACD: Setting up a Virtual Organisation

- **Setting up virtual organizations (VOs) for a specific purpose.**
- Requires acquiring certificate for the VO group in the usual involved way by an expert-user (the admin of the group).
- Users don't know or care about this at all.



# The Application Hosting Environment

AHE is a tool for building Science Gateways – currently used at UCL to provide a gateway for our users

- Based on the idea of applications as stateful RESTful services
- Lightweight hosting environment for running unmodified applications on grid and local resources
- Community model: expert user installs and configures an application and uses the AHE to share it with others
- Simple clients with very limited dependencies
- No intrusion onto target grid resources

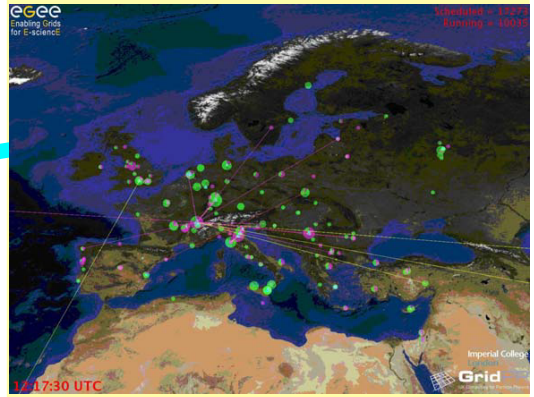
# AHE: Bridging the Gap

UCL

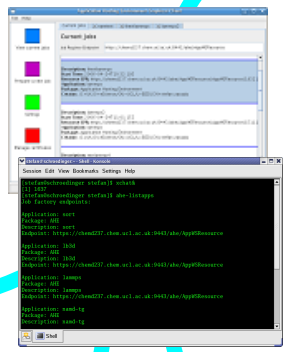
Local resources

QCG Computing

EGI




GridSAM

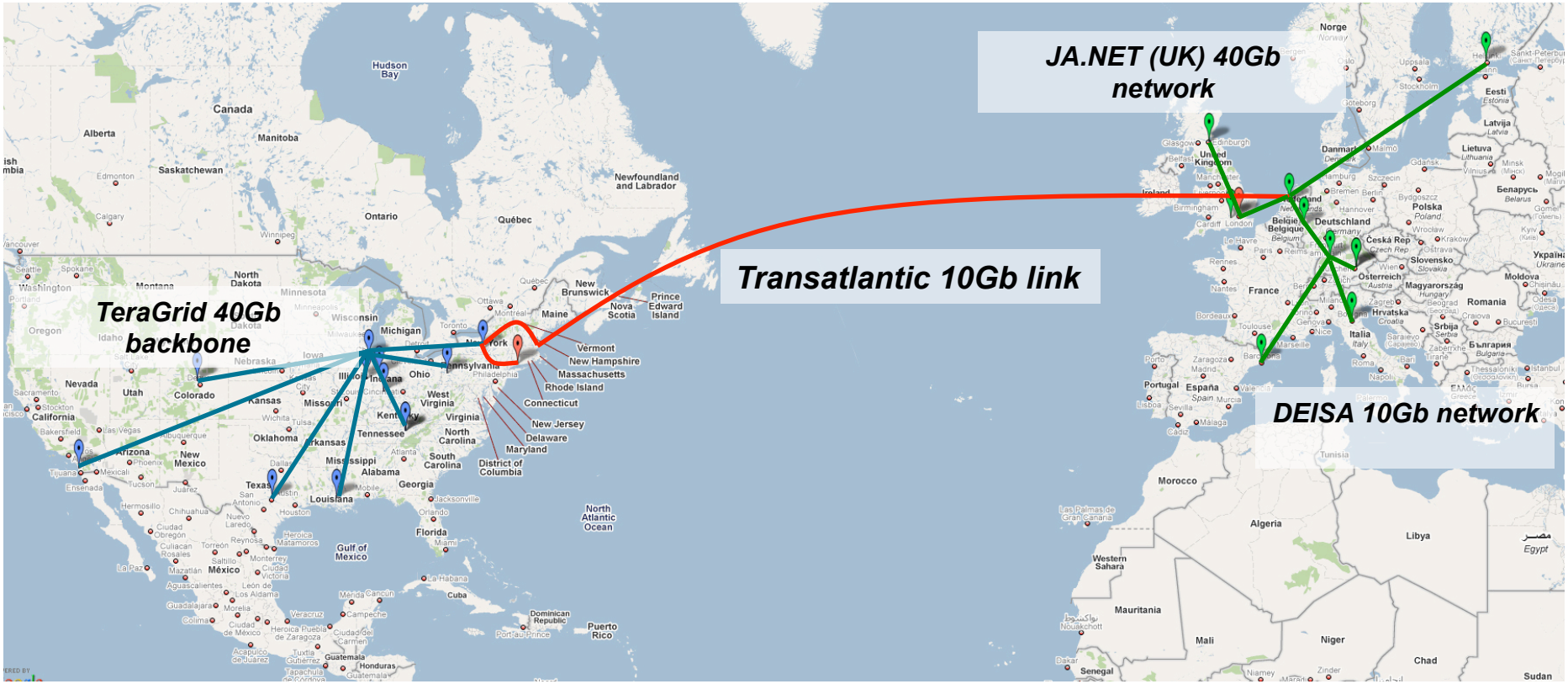


XSEDE


Globus

UNICORE

PRACE


JA.NET (UK) 40Gb network
Transatlantic 10Gb link
TeraGrid 40Gb backbone
DEISA 10Gb network

# AHE & ACD Usability Study

- Usability: we have completed a comprehensive usability study that involved:
  - Comparing AHE+ACD (GUI), AHE (GUI) and UNICORE GUI, AHE command line and Globus TK command line
  - 40 users from different UCL departments (Physics, Computer Science, Medical school, Business School, Chemistry, Cancer Institute, Law School)
  - Task: run a simulation on Grid (NGS) using the above middlewares and use credentials given to users (username/ password, X509 Certificate)
  - Result: AHE+ACD scored best in respect of:
    - Time needed to run the task
    - Ease of configuring the tool
    - Ease of running the whole task.

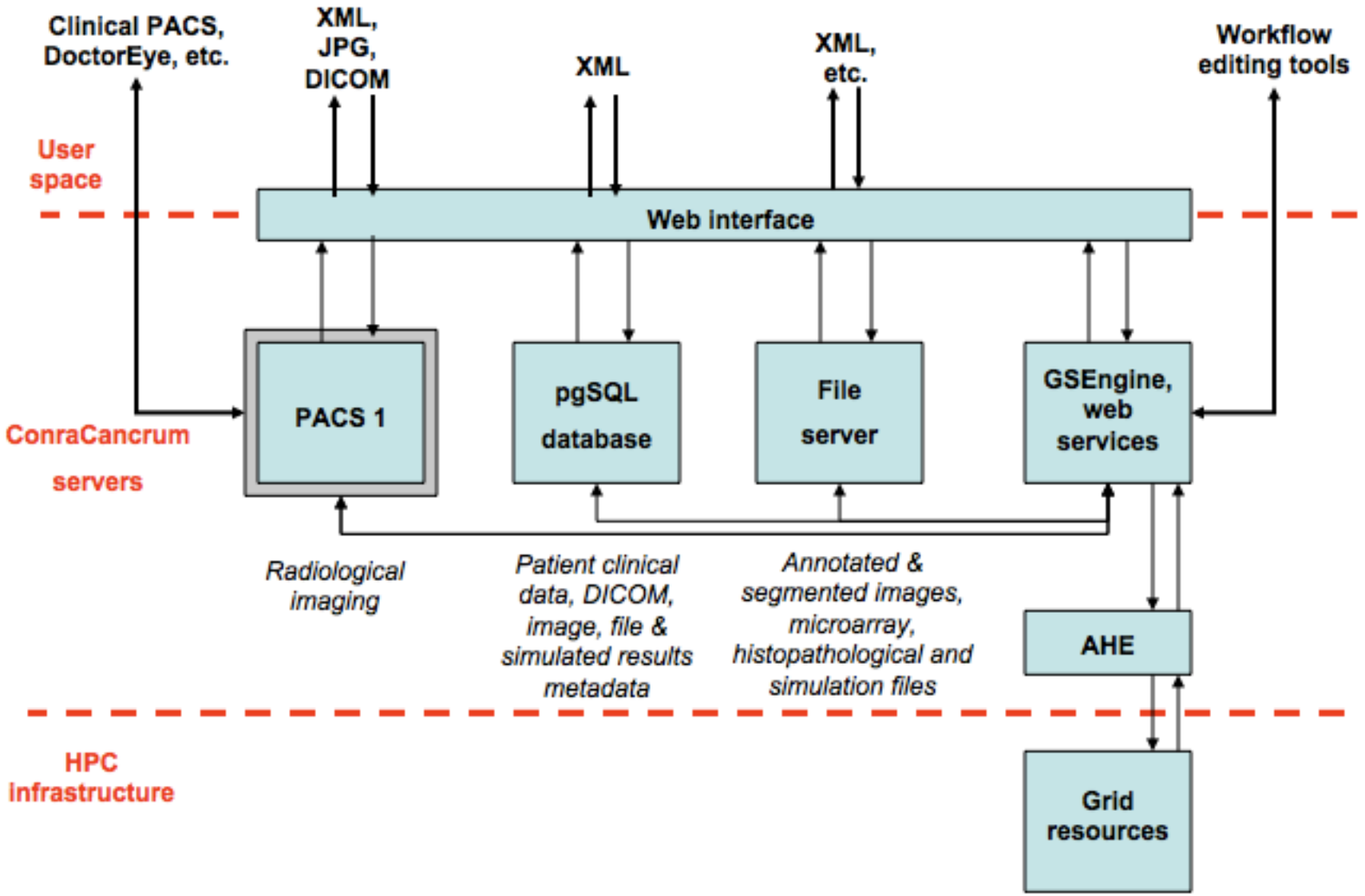
S. J. Zasada, A. N. Haidar, and P. V. Coveney, “On the Usability of Grid Middleware and Security Mechanisms”. *Phil. Trans. R. Soc. A* , 2011, 369 (1949) 3413-3428; doi:10.1098/rsta.2011.0131

# Individualized MEdiciNe Simulation Environment - IMENSE

- Aims
  - Central integrated repository of patient data for project clinicians & researchers
  - Storage of and audit trail of computational results
  - Interfaces for data collection, editing and display
  - Provides a data environment for
    - Integration of multi-scale data
    - Decision support environment for clinicians
- Critical factors for success and longevity
  - Use Standards and Open Source solutions
  - Use pre-existing EU FP6/FP7 solutions and interaction with VPH-NoE Toolkit

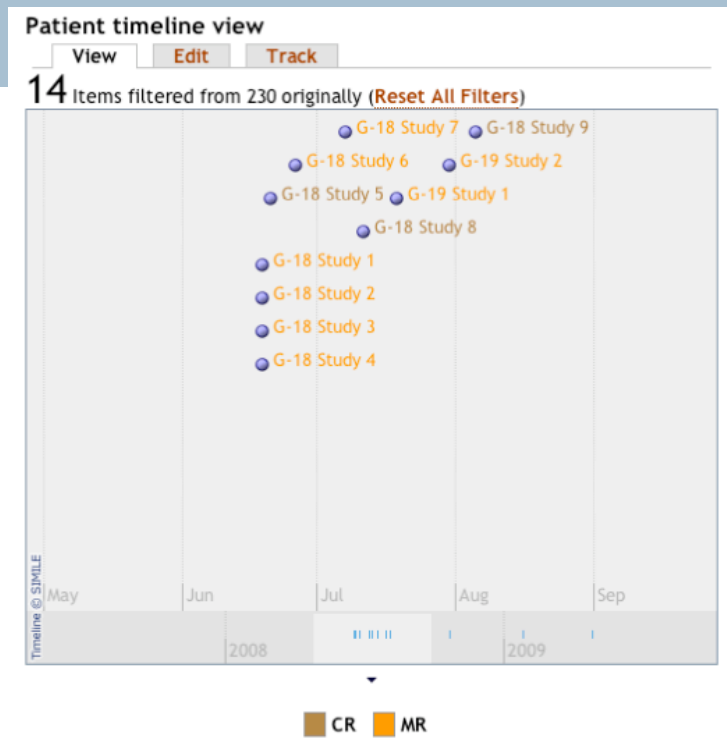
S. J. Zasada et al., "IMENSE: An e-Infrastructure Environment for Patient Specific Multiscale Modelling and Treatment, Journal of Computational Science, In Press, Available online 26 July 2011, ISSN 1877-7503, DOI: 10.1016/j.jocs.2011.07.001.

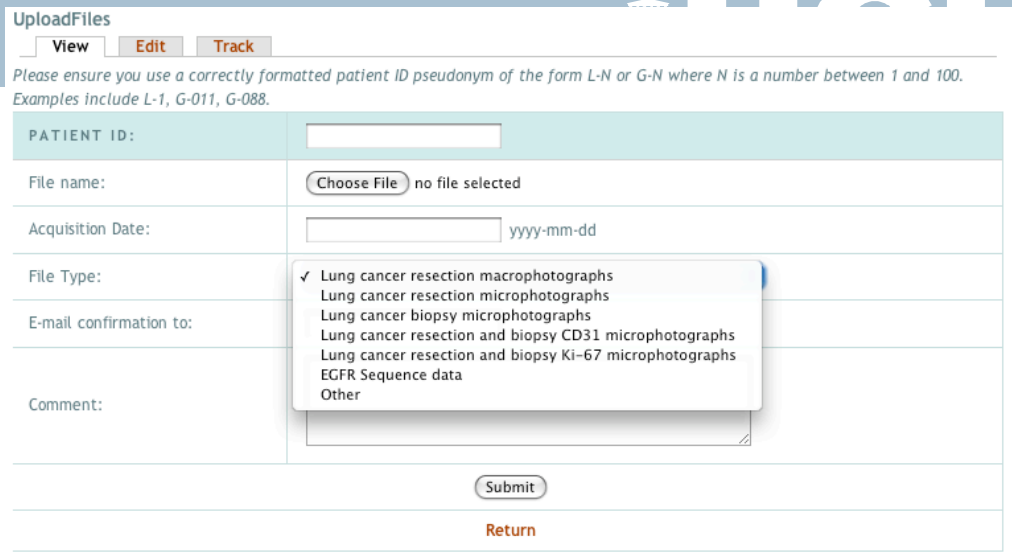
# IMENSE: Integrating the components

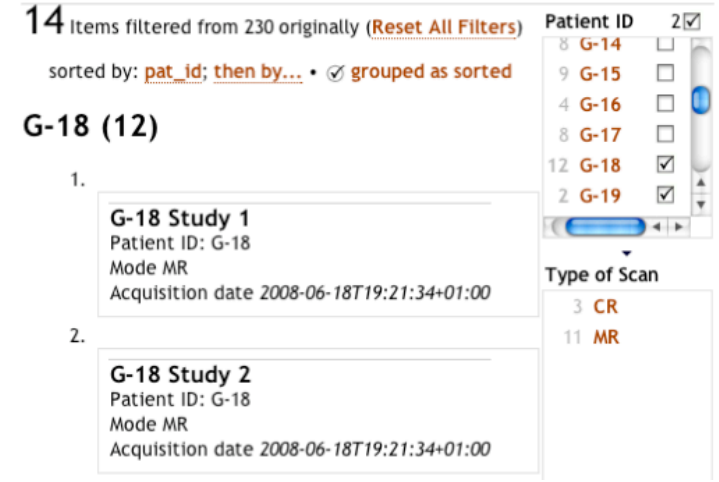


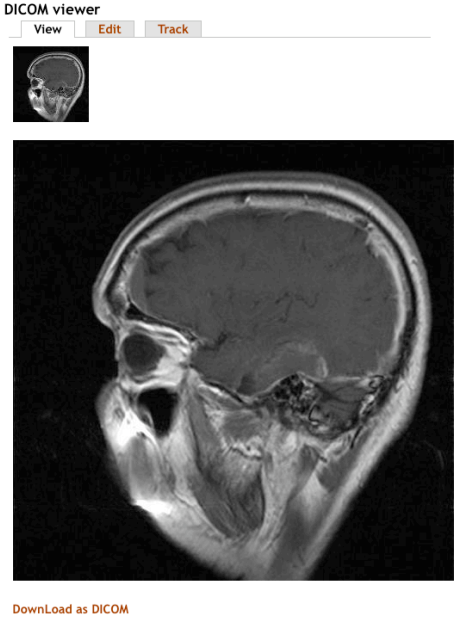

S. J. Zasada et al., "IMENSE: An e-Infrastructure Environment for Patient Specific Multiscale Modelling and Treatment, Journal of Computational Science, In Press, Accepted Manuscript, Available online 26 July 2011 ISSN 1877-7503, DOI: 10.1016/j.jocs.2011.07.001.

# IMENSE: Interacting with data

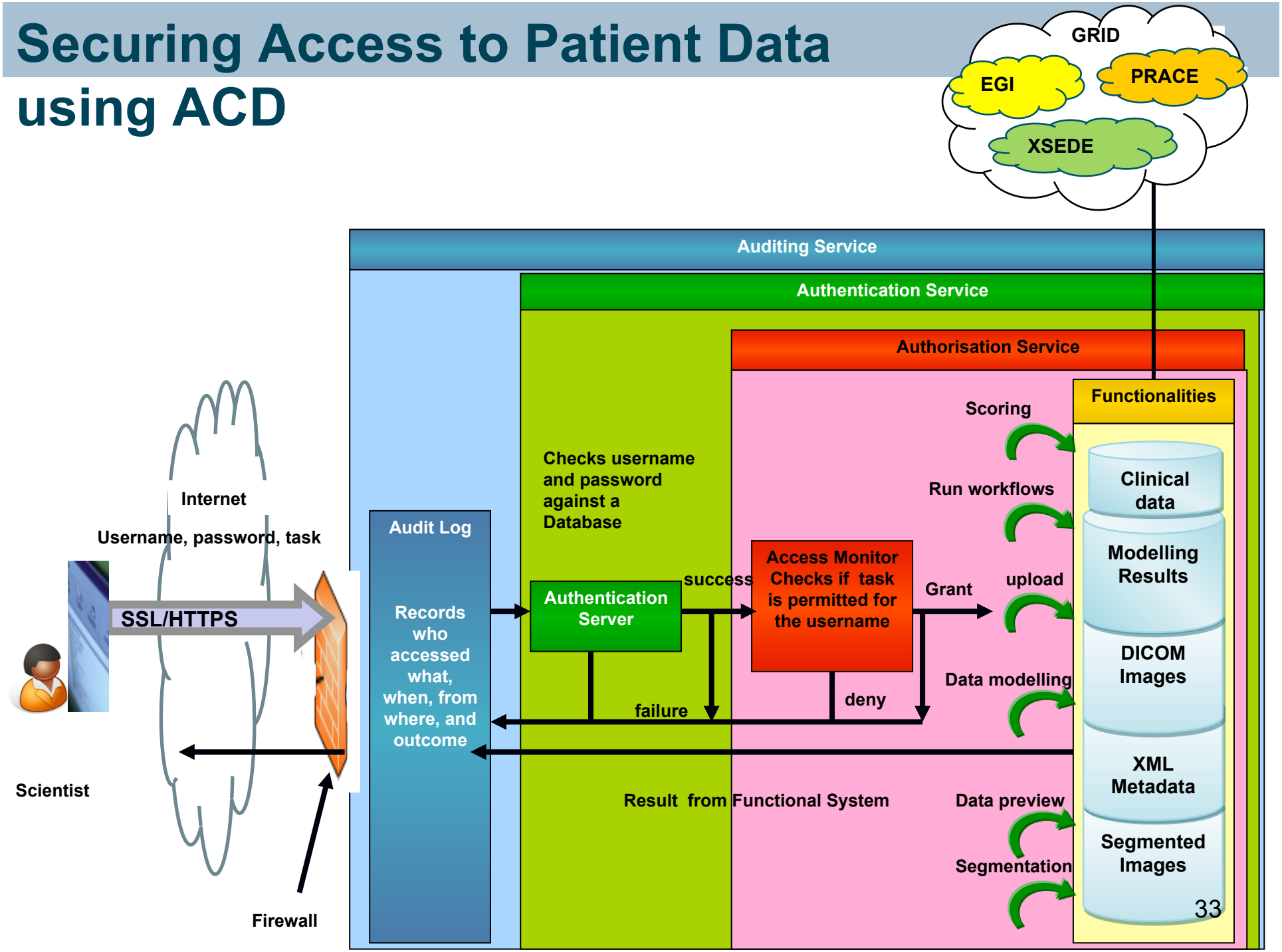


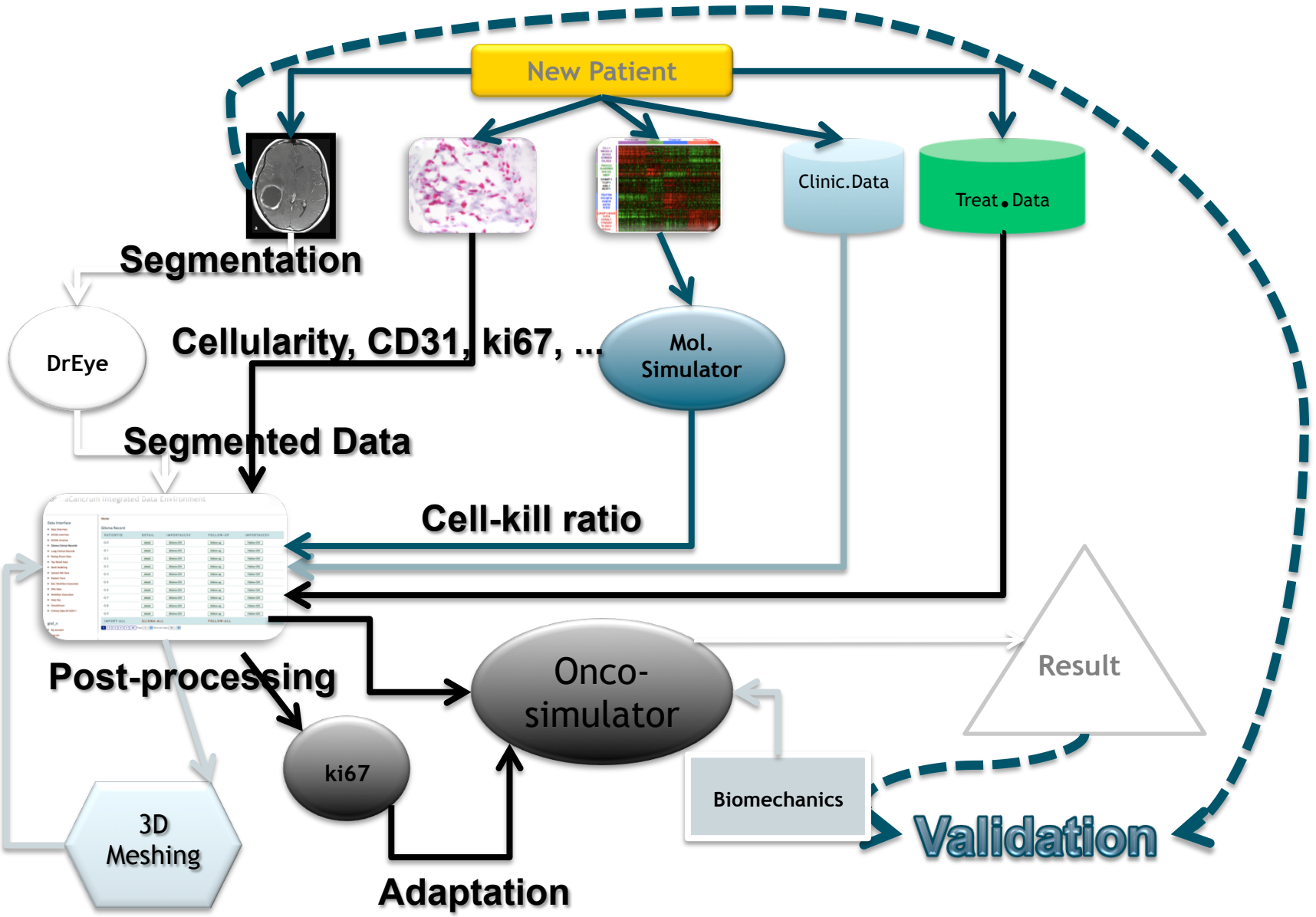




# Securing Access to Patient Data using ACD



# Glioma Workflow Scenario using various patient data stored in IMENSE



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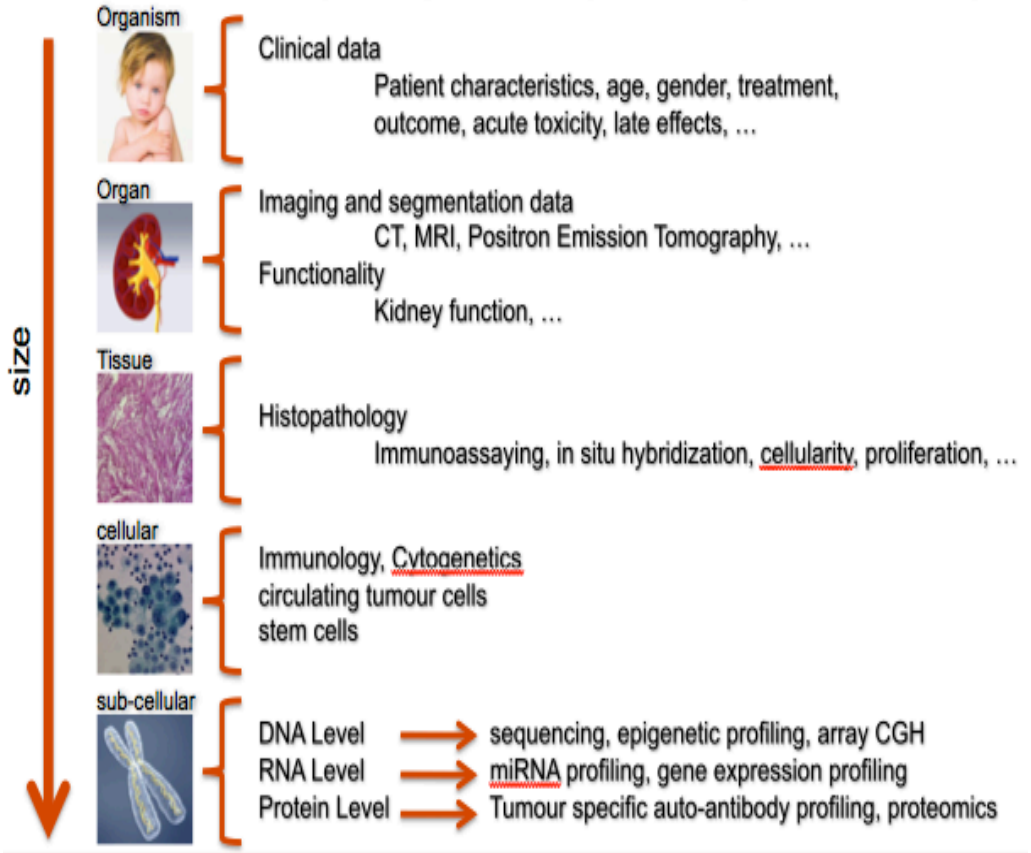
# Virtual Physiological Human (VPH)

- €207M initiative in EU-FP7
- Aims
  - Enable collaborative investigation of the human body across all relevant scales.
  - Introduce *multiscale* methodologies into medical and clinical research
- The VPH framework is:
  - Descriptive
  - Integrative
  - Predictive

**Organism**
**Organ**
**Tissue**
**Cell**
**Organelle**
**Interaction**
**Protein**
**Cell Signals**
**Transcription**
**Gene**
**Molecule**

Virtual Physiological Human
network of excellence

# Large scale data & computing




- Models are built for use in clinical decision support
  - results are needed in a timely fashion.
- It is necessary to have the possibility of seamlessly "plugging in" resources for parallel and large scale computing "here and now"
  - petascale computing is needed to perform e.g.:
    - drug binding affinity determination
    - blood flow through tumours
- Gratis via VPH-NoE supervised VPH Virtual Community allocations of time on PRACE

**Seamless access and integration of distributed, heterogeneous data in a data warehouse repeatedly over time (≈ 200 GB / patient and time point)**

# VPH NoE

Specifically, the VPH NoE:

- ***Has identified user needs, defined standards, ontologies and applications; in the advanced stage of developing the VPH ToolKit***
- Is in process of developing VPH training activities and materials: Joint advanced degree programme, interdisciplinary study groups, focused journal issues, textbook
- Is providing research/news dissemination services and international EU/international networking
- VPH2012 Integrative Computational Biomedicine, 18-20 Sept 2012

Project Coordinator: Vanessa Díaz-Zuccarini / Miriam Mendes (UCL)

PI & Scientific Coordinator: Peter Coveney (UCL)

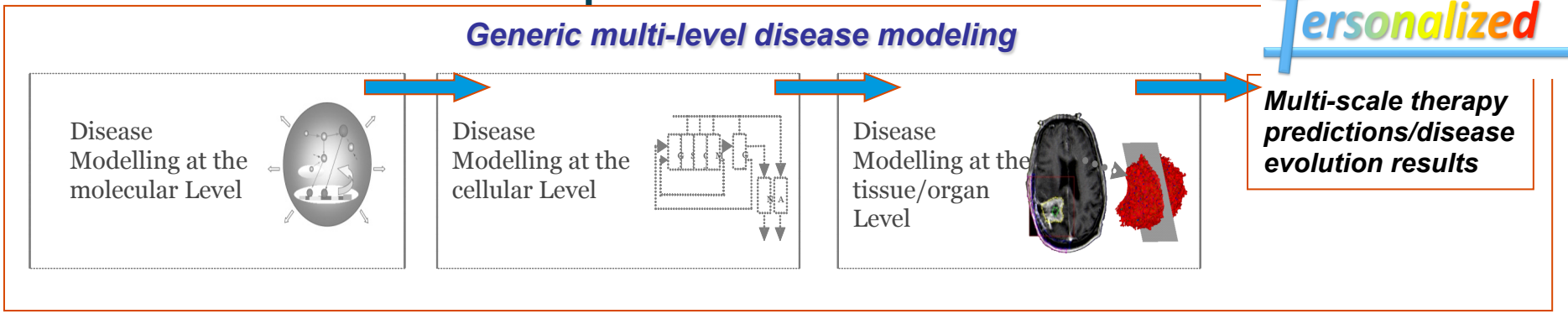
http://www.vph-noe.eu

# Virtual Physiological Human

- 30 projects: 1 NoE, 5 IPs, 22 STREPs, 3 CAs.
- 12 new FP7 projects in 2011

***"a methodological and technological framework that, once established, will enable collaborative investigation of the human body as a single complex system ..."***

# P-MEDICINE: From data sharing and integration via VPH models to personalized medicine

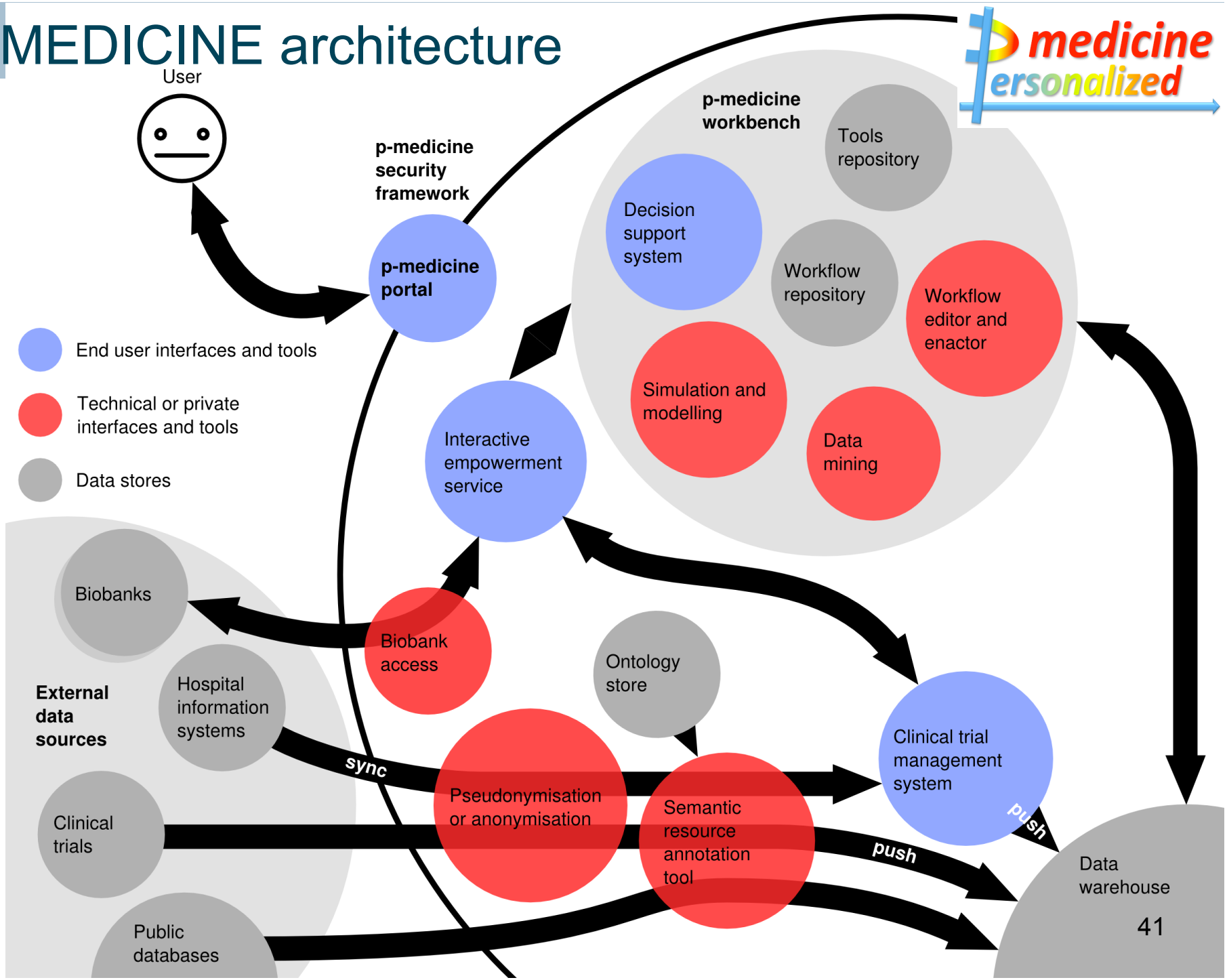



- Predictive disease modelling
- Exploiting the individual data of the patient in federated data warehouse
- Optimization of cancer treatment (Wilms tumor, breast cancer and acute lymphoblastic leukemia)
- Infrastructure supports:
  - generic seamless, multi-level data integration
  - VPH-specific, multi-level, cancer data repository
  - model validation and clinical translation through trials
- Scalable for any disease - as long as:
  - predictive modeling is clinically significant in one or more levels
  - development of such models is feasible

http://www.p-medicine.eu/

***Led by a clinical oncologist - Prof Norbert Graf* €13M, 2011-2013, EU FP7**

# P-MEDICINE architecture



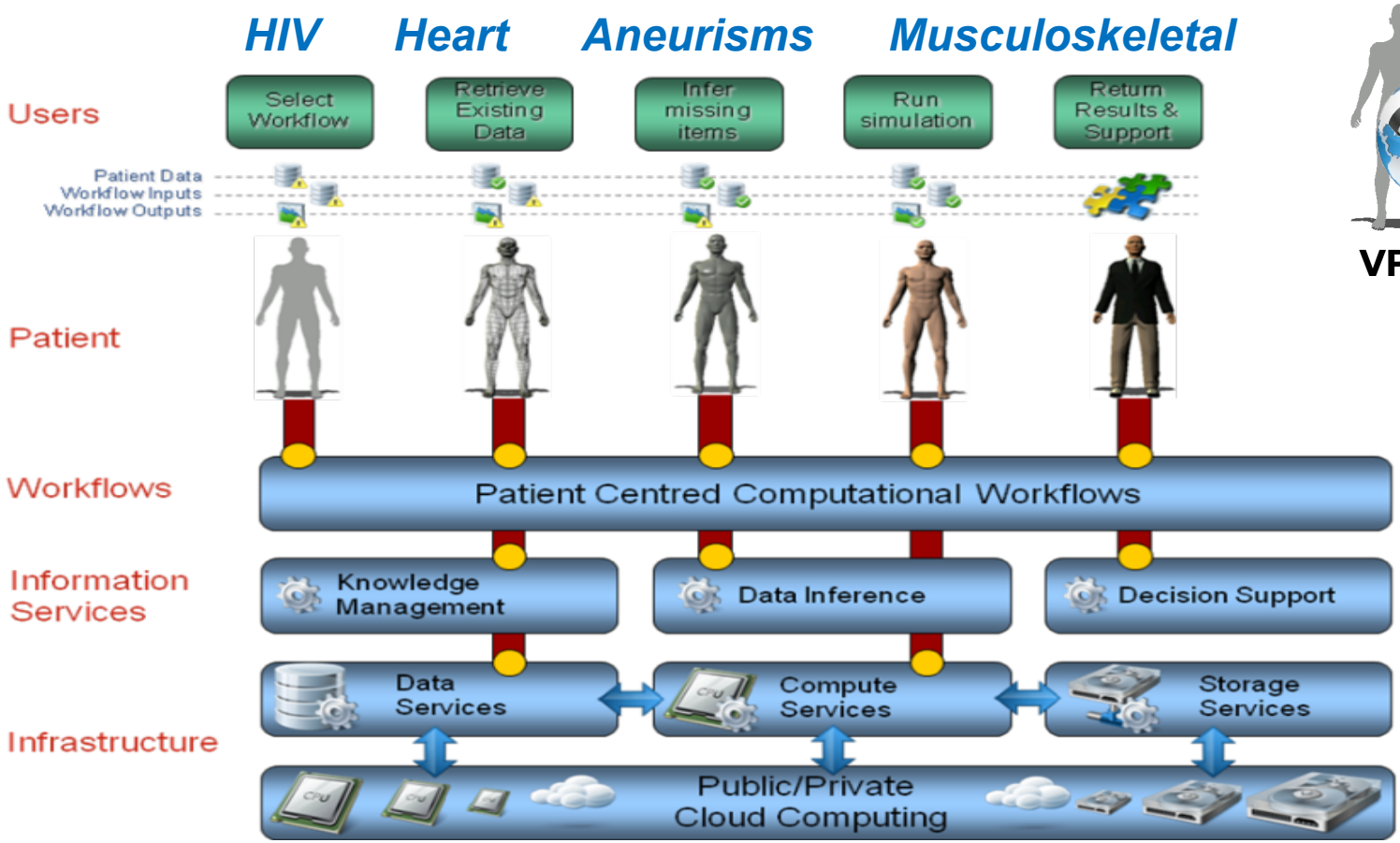
# VPH-SHARE overview

- VPH-SHARE is developing the organisational fabric and integrating the optimised services to:
  - expose and share patient data (imaging, clinical, biomedical signals)
  - jointly develop multiscale models for the composition of new VPH workflows from @neurIST, euHeart, VPHOP, and Virolab projects
  - facilitate collaborations within the VPH community
  - evaluate the effectiveness and fitness-for -purpose of Data and Compute Cloud platforms for biomedical applications

- The project focuses on a key bottleneck: the interface with the wealth of data from medical research infrastructures and from clinical processes.

- Led by Rod Hose, Sheffield, UK (http://vph-share.org/)

# VPH-Share Overview




**VPH*Share***

***VPH-Share will provide the organisational fabric realised as a series of services, offered in an integrated framework, to expose and to manage data, information and tools, to enable the composition and operation of new VPH workflows and to facilitate collaborations between the members of the VPH community.***



**€11M, 2011-2015, EU FP7 – Promotes cloud technologies**

# Bridging gaps between Bioinformatics and Medical informatics

**Bioinformatics**
in biomedical research
(molecular, “omics”,
systems biology)

HEAVY BARRIERS - MUTUAL IGNORANCE

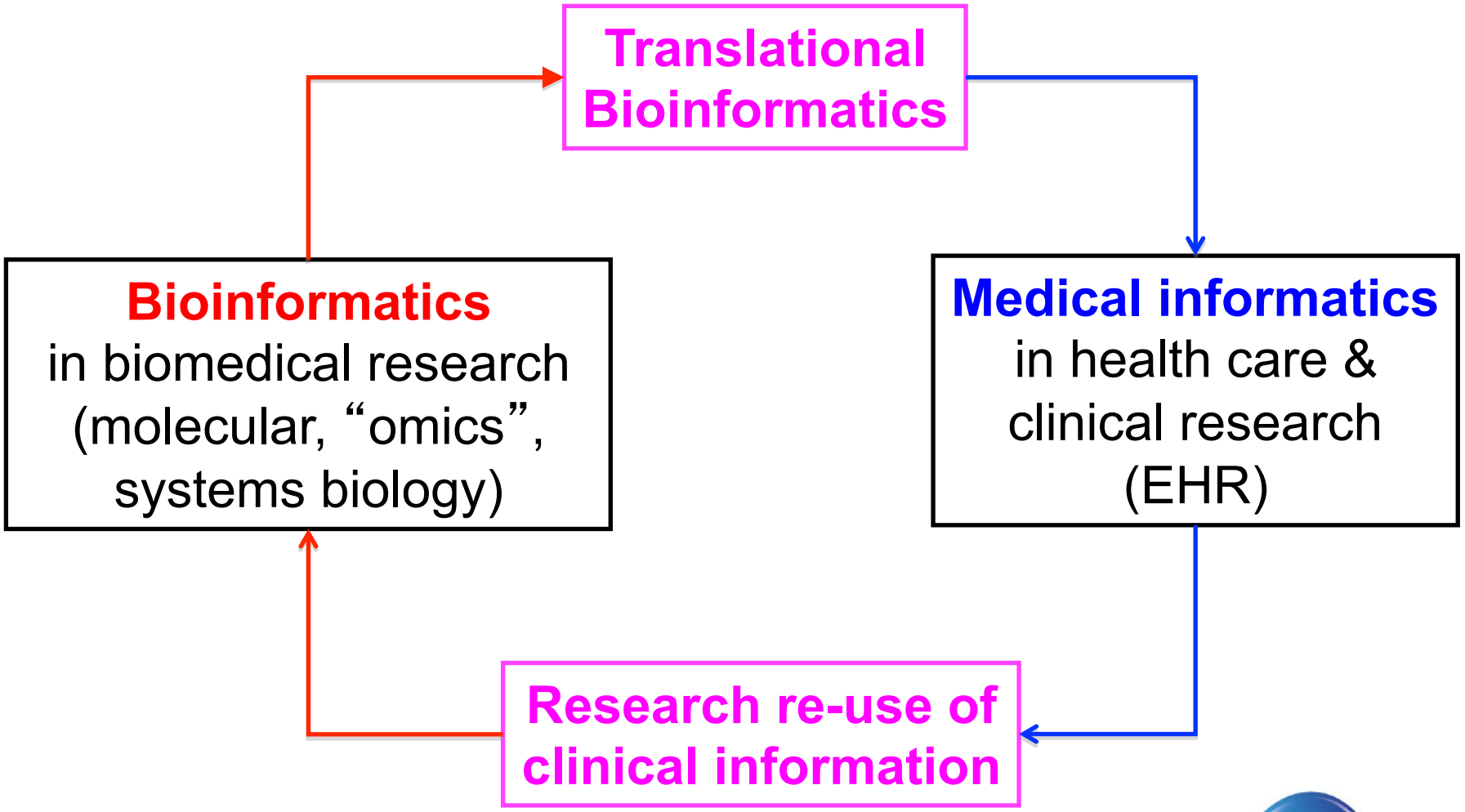
**Medical informatics**
in health care &
clinical research
(EHR)

€1M EU VPH FP7 project, *devoted to the organisation and execution of a series of activities to support the field of Biomedical Informatics*

INBIOMEDvision

**www.inbiomedvision.eu**

# Bridging gaps between Bioinformatics and Medical Informatics




INBIOMEDvision

# Overview

- The UCL Centre for Computational Science
- Computational Biomedicine Case Studies
- Medical Data Storage and Security issues
- The Virtual Physiological Human initiative
- EU e-Infrastructure Projects for Biomedical Data Processing
- Conclusions

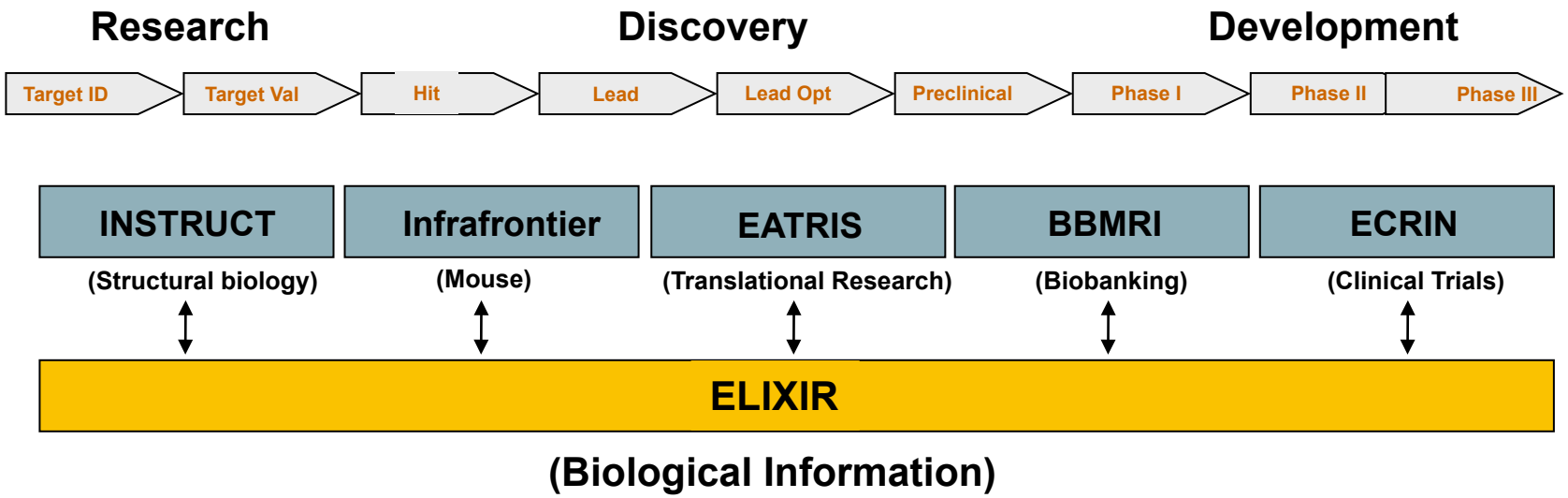
# ELIXIR: European life-science infrastructure for biological information

- The mission of ELIXIR is to construct and operate a sustainable infrastructure for biological information in Europe to support life science research and its translation to medicine and the environment, the bio-industries and society
- Five year EU-funded collaborative project, 31 partners, €4.5 million funding.
- Benefits
  - Optimising access to and exploitation of life-science data.
  - Ensuring longevity of the data and protecting investments already made in research which collected the data.
  - Increasing the competence and size of the already-large user community by strengthening national efforts in training and outreach

http://www.elixir-europe.org/

# ELIXIR

- ELIXIR underpins other developing European Biomedical Science projects across the research and discovery spectrum.




**Slide courtesy** of Ewan Birney

# ELIXIR: Sustainable European Infrastructure

**Slide courtesy** of Ewan Birney

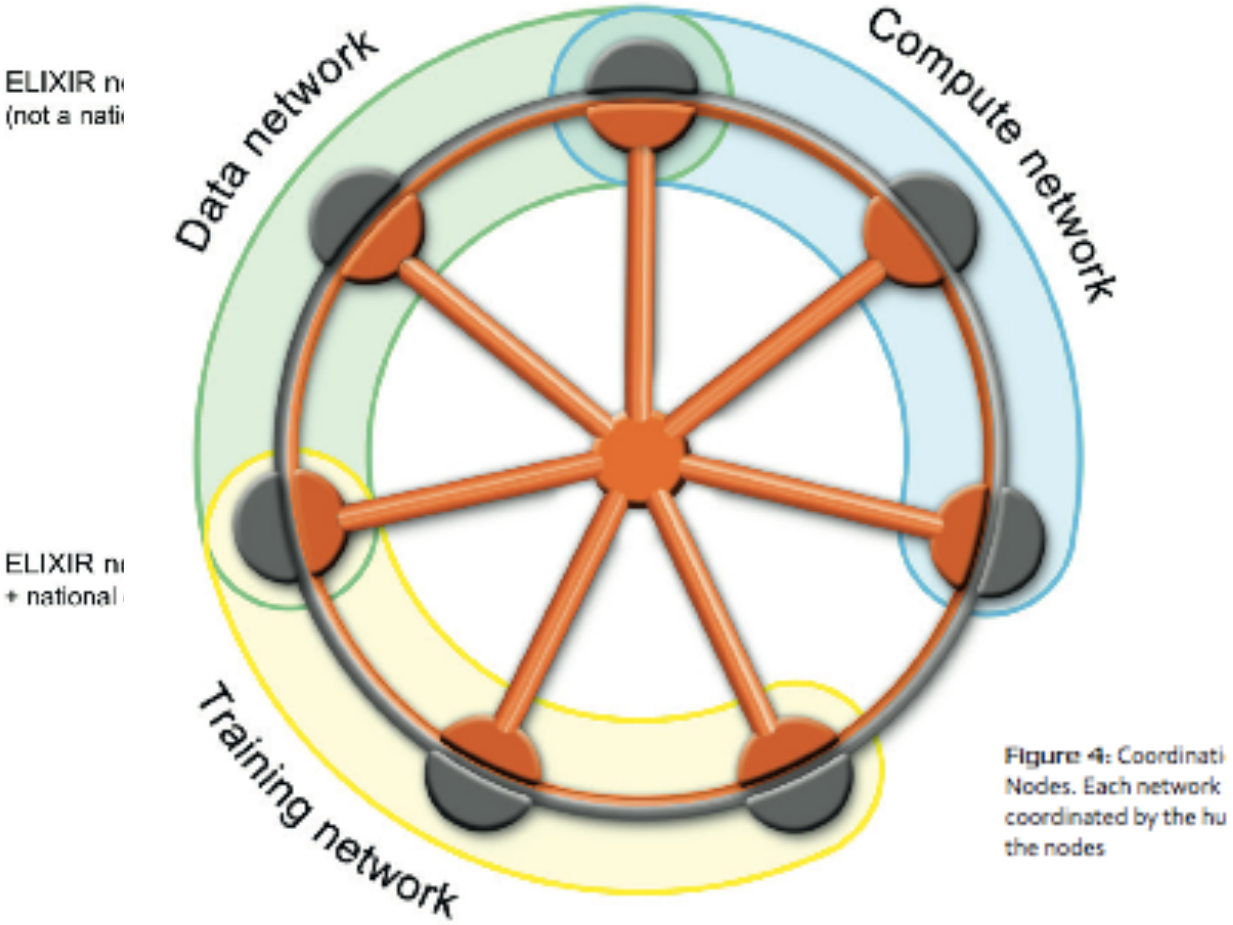



Figure 4: Coordinati
Nodes. Each network
coordinated by the hu
the nodes

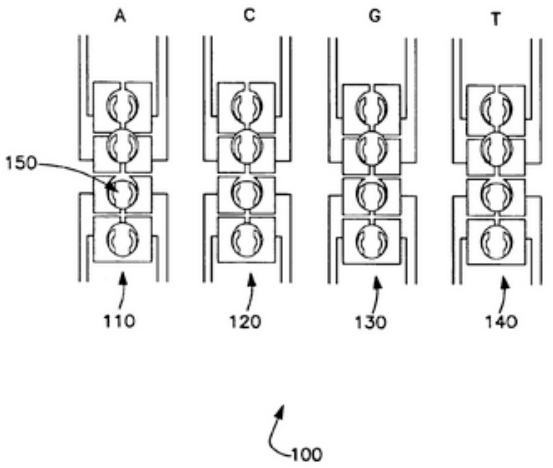
# New Machines


illumina



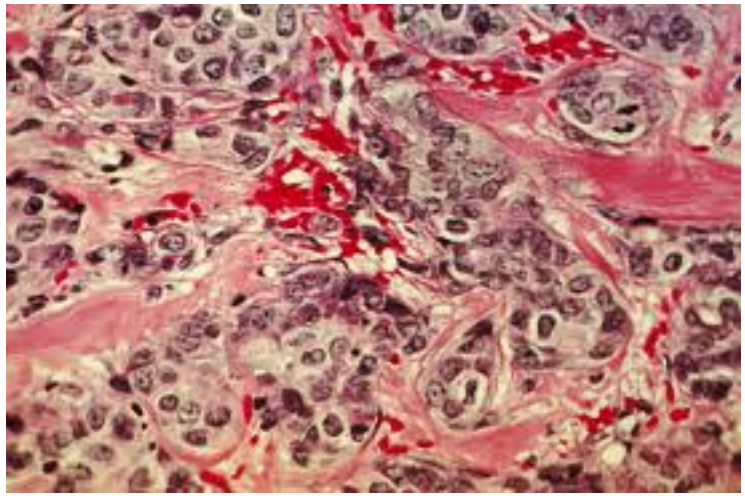
AB App Bios

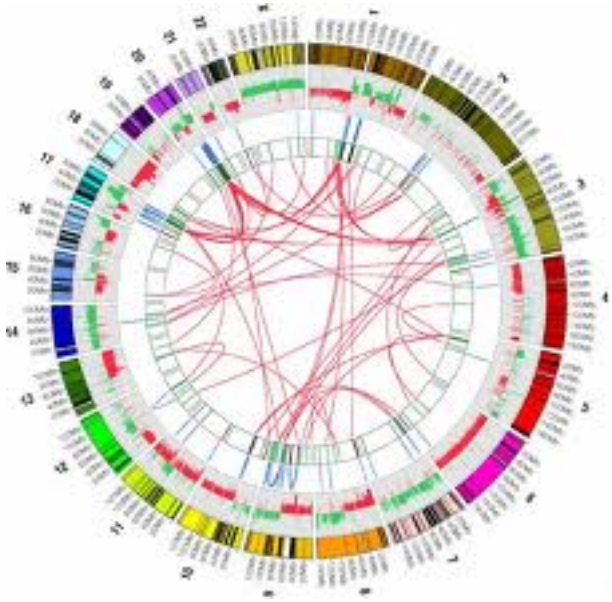
**1 Human Genome in:**
**~5 years (2001)**
**2 years (2004)**
**4 days (Jan 2008)**
**16 Hours (Oct 2008)**
**3 Hours (Nov 2009)**
**6 minutes (Now!)**




**Slide courtesy** of Ewan Birney

International Cancer Genome Consortium





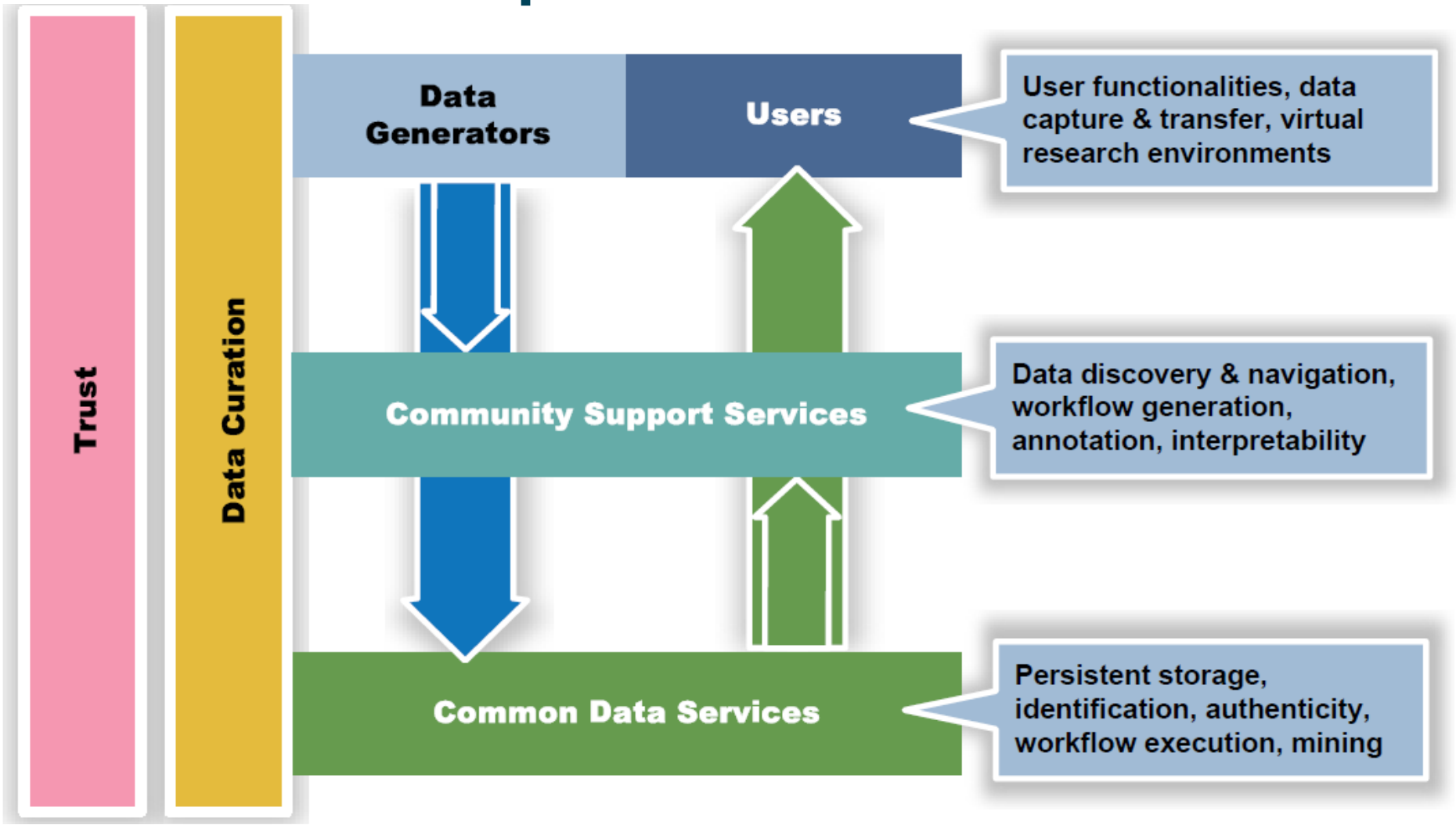
**Committed – 20,000 high coverage genomes in 5 years for research**
**~300,000 new cases/year in UK**

# EUDAT


- Aims:
  - To deliver a Collaborative Data Infrastructure (CDI) with the capacity and capability for meeting future researchers' needs in a flexible and sustainable way, across geographical and disciplinary boundaries
- Total Budget
  - Total: €10 M over 3 years
  - 55% EC funded, 45% self-funded through financial engineering
- User communities
  - Biomedical Sciences: ELIXIR
  - Social Sciences: CLARIN
  - Environmental Sciences: Lifewatch, EPOS
  - High Energy Physics
  - Climate: ENES
  - Virtual Physiological Human (VPH)

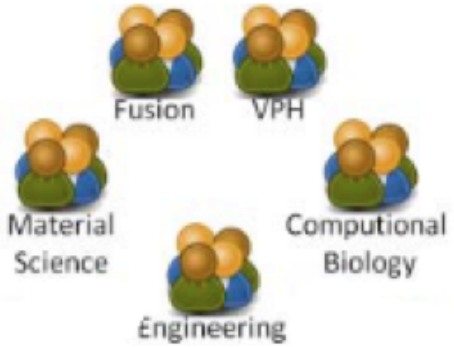
http://www.eudat.eu/

# Towards a European Data Infrastructure




- **Aims at 24/7 service provision within first three years, and sustained service beyond**


- Goal: To make multiscale applications possible on European production e-Infrastructures.
- Duration: Oct. 2010 – Sept. 2013.
- 5 application domains within the project,
  - + cooperation with external communities.

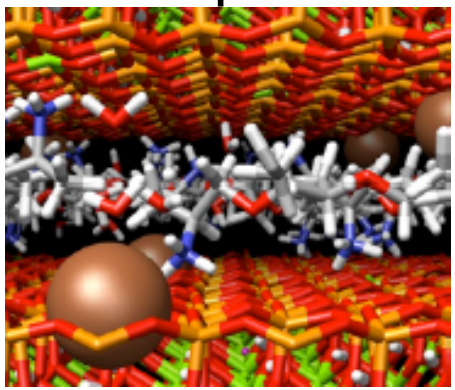
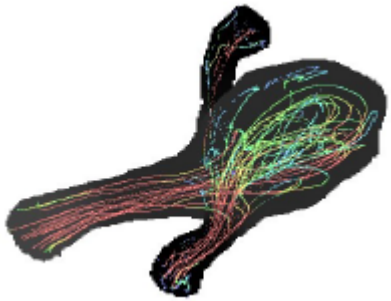


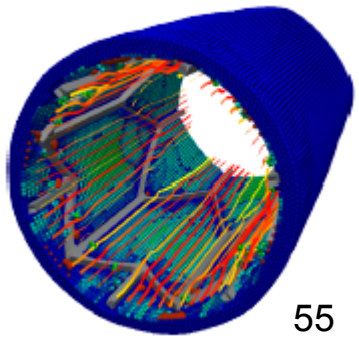

- EU FP7 project with partners throughout Europe.
- http://www.mapper-project.eu

***Distributed Multiscale Computing workshop at this conference!***

# Simulating Complex Systems

- Physical systems are often inherently multiscale.
- Micro- and mesoscopic processes influence the macroscopic behaviour of the system, and *vice versa*.
- Simulating all processes in a complex system with a single code is often an impossible endeavour.
  - High resolution needed to resolve microscopic processes.
  - Microscopic accuracy + macroscopic problem size => prohibitive computational and storage demands.



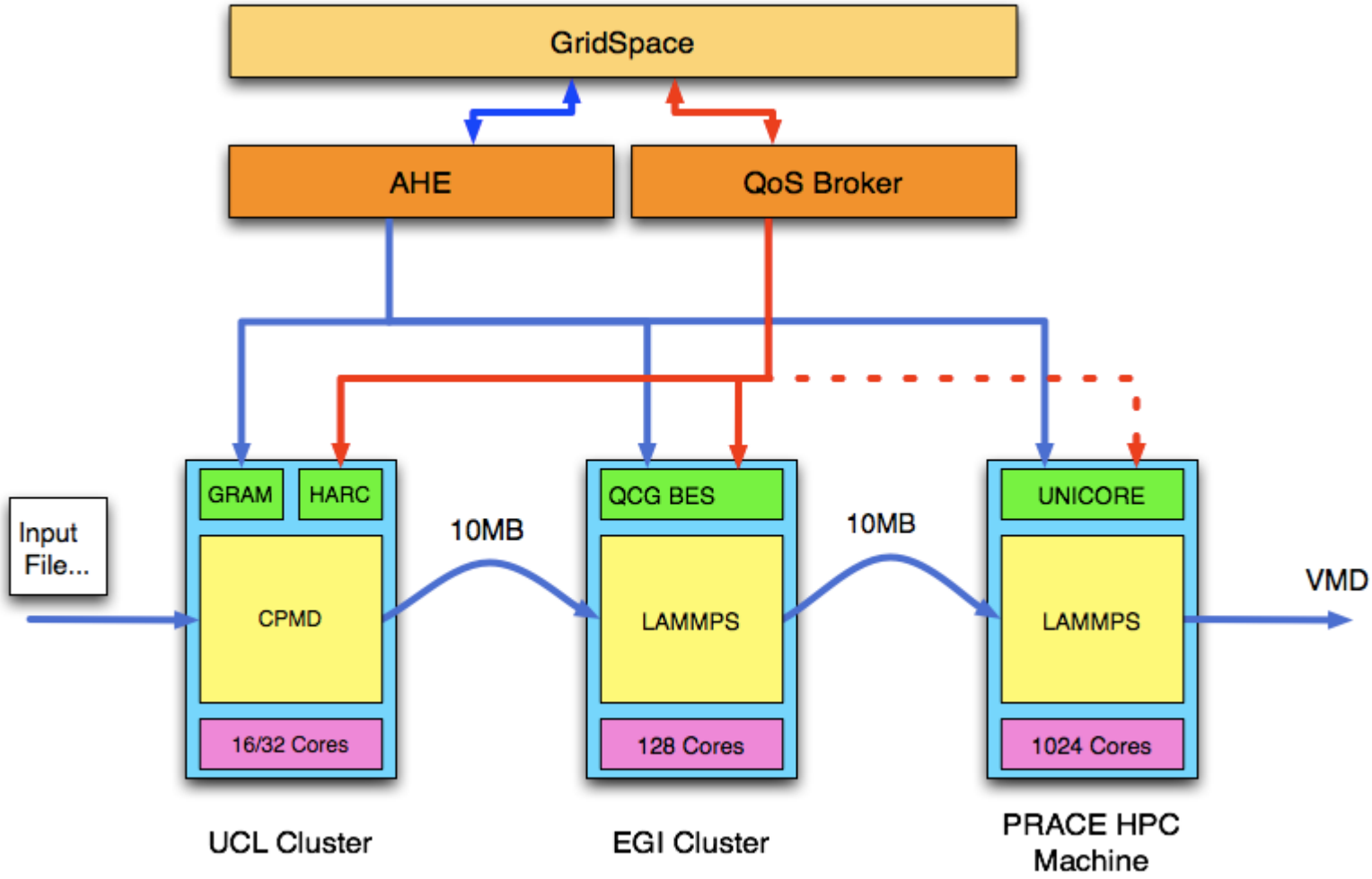
# Coupling methods


- Two-way “tight” coupling between subcodes.
  - e.g. continuum-particle hybrid coupling.
    - R. Delgado-Buscalioni and P. V. Coveney, Phys. Rev. E 67, 046704 (2003)
  - Typically performed using coulding methods
- One-way “loose” coupling between subcodes.
  - Typically performed using workflow managers.

    e.g. GridSpace (http://dice.cyfronet.pl/gridspace/)
- Needs seamless interoperation of “high” and “low” end resources (e.g. PRACE, EGI) with data (EUDAT) and networks (GEANT)

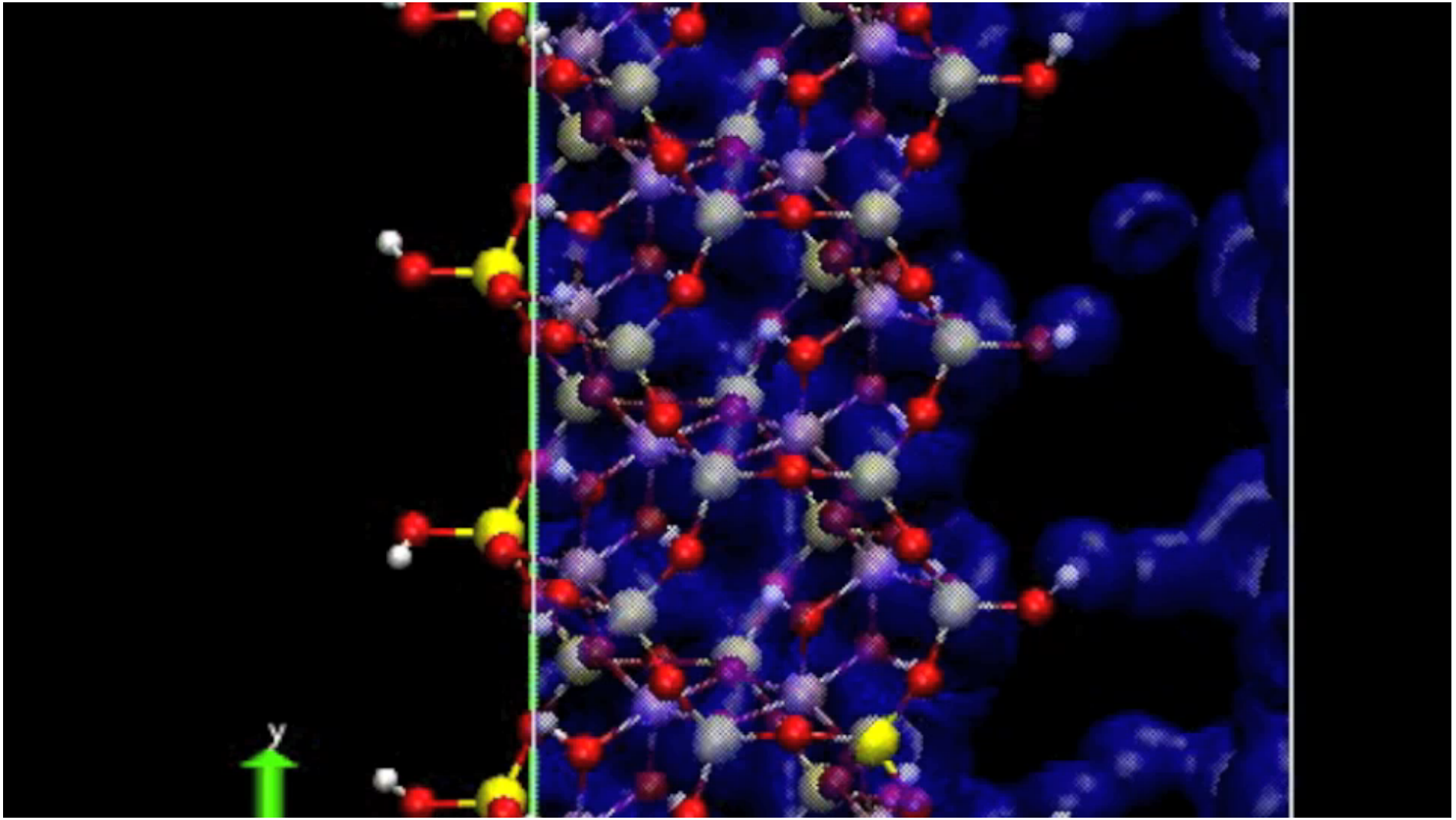
# Infrastructure Used

## Example: Multiscale modelling of cancer drugs and targets




**Additional higher temperature replicas will improve sampling.**

# MAPPER Simulation Workflow




**Multiscale modelling and simulation of clay-polymer nanocomposites**

# MAPPER Computing e-Infrastructure

# The CRESTA Project


- Three year EU-funded collaborative project, 13 partners, €8.5 million funding
  - Collaborative Research into Exascale Systemware, Tools and Applications
  - Project coordinator: EPCC at The University of Edinburgh
- CRESTA has a very strong focus on exascale software challenges
- The hardware partner is Cray
- Applications represent broad spectrum from science and engineering
- CRESTA will compare and contrast incremental and disruptive solutions to Exascale challenges

http://cresta.epcc.ed.ac.uk/

# Consortium & Applications

- Leading European HPC centres
  - EPCC, HLRS, CSC, PDC
- A world leading vendor
  - Cray
- World leading tool providers
  - TUD (Vampir), Allinea (DDT)

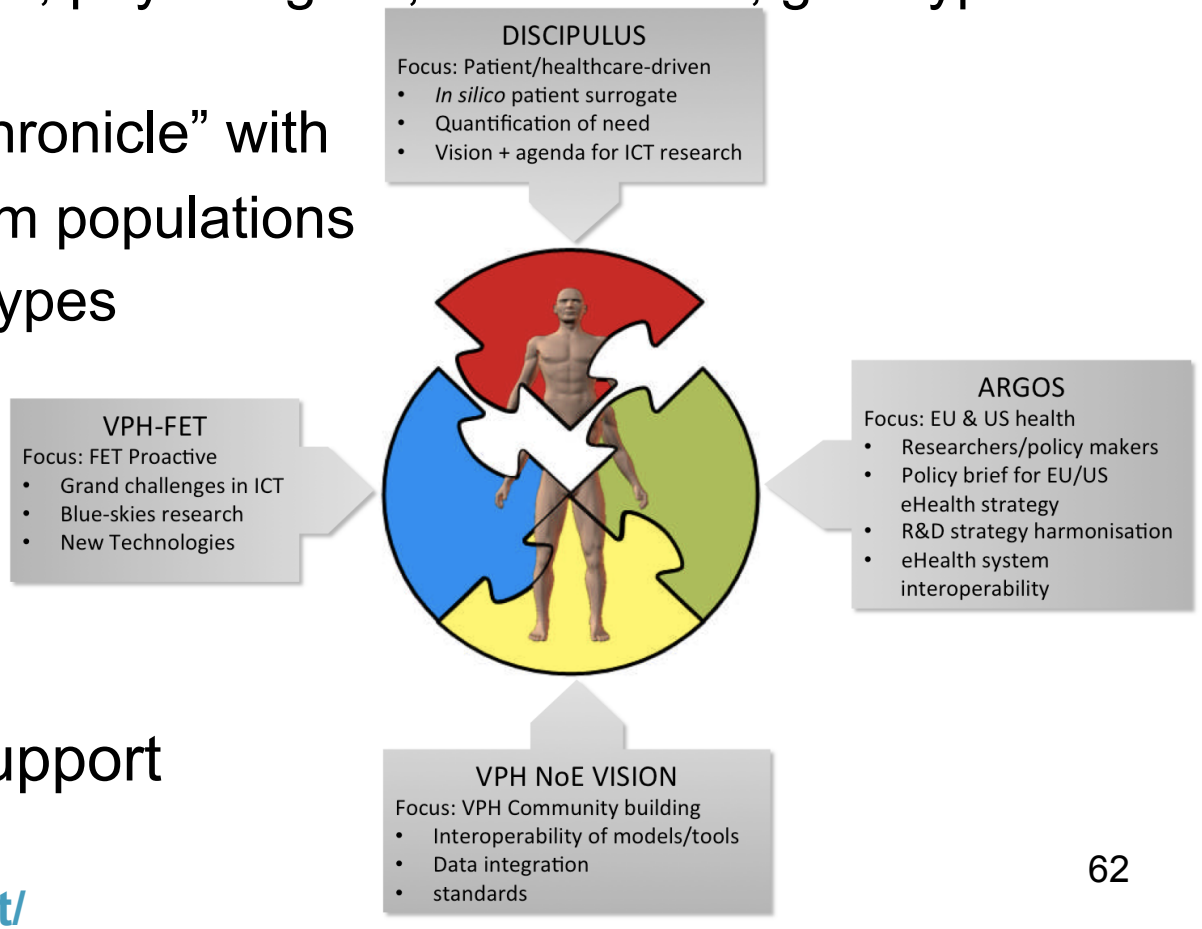

- Exascale application owners and specialists
  - ABO, JYU, UCL, ECMWF, ECP, DLR

| Application | Grand challenge | Partner responsible |
|---|---|---|
| GROMACS | Biomolecular systems | KTH (Sweden) |
| ELMFIRE | Fusion energy | ABO (Finland) |
| **HemeLB** | **Virtual Physiological Human** | **UCL (UK)** |
| IFS | Numerical weather prediction | ECMWF (International) |
| OpenFOAM | Engineering | EPCC / HLRS / ECP |
| Nek5000 | Engineering | KTH (Sweden) |

# DISCIPULUS:

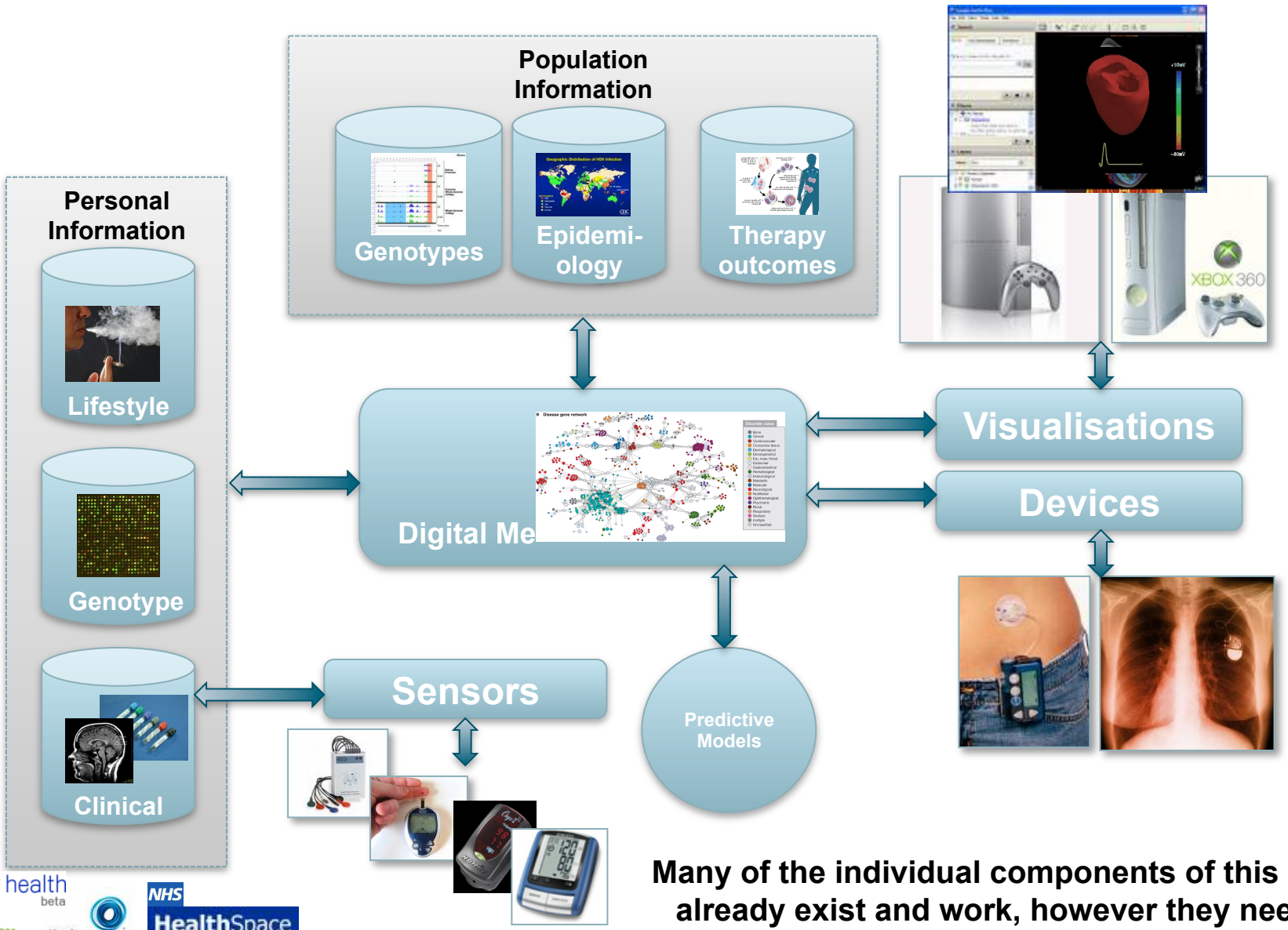
## A vision of future healthcare

- "The Digital Patient", € 1.4M, EU FP7, led by Vanessa Diaz, leading to Road Map in the next 15 months.
- Personalised, Predictive, Integrative...
- An integrated anatomical, physiological, biochemical, genotypical model of *me*
- Integrates *my* health "chronicle" with models derived from populations with similar phenotypes
- Used for:
  - Patient education
  - Management of chronic diseases
  - Clinical decision support




http://www.digital-patient.net/

# Digital Me




Google health beta
MAYO CLINIC Health Manager
Microsoft HealthVault
NHS HealthSpace

**Many of the individual components of this figure already exist and work, however they need to be integrated**

# IT Future of Medicine

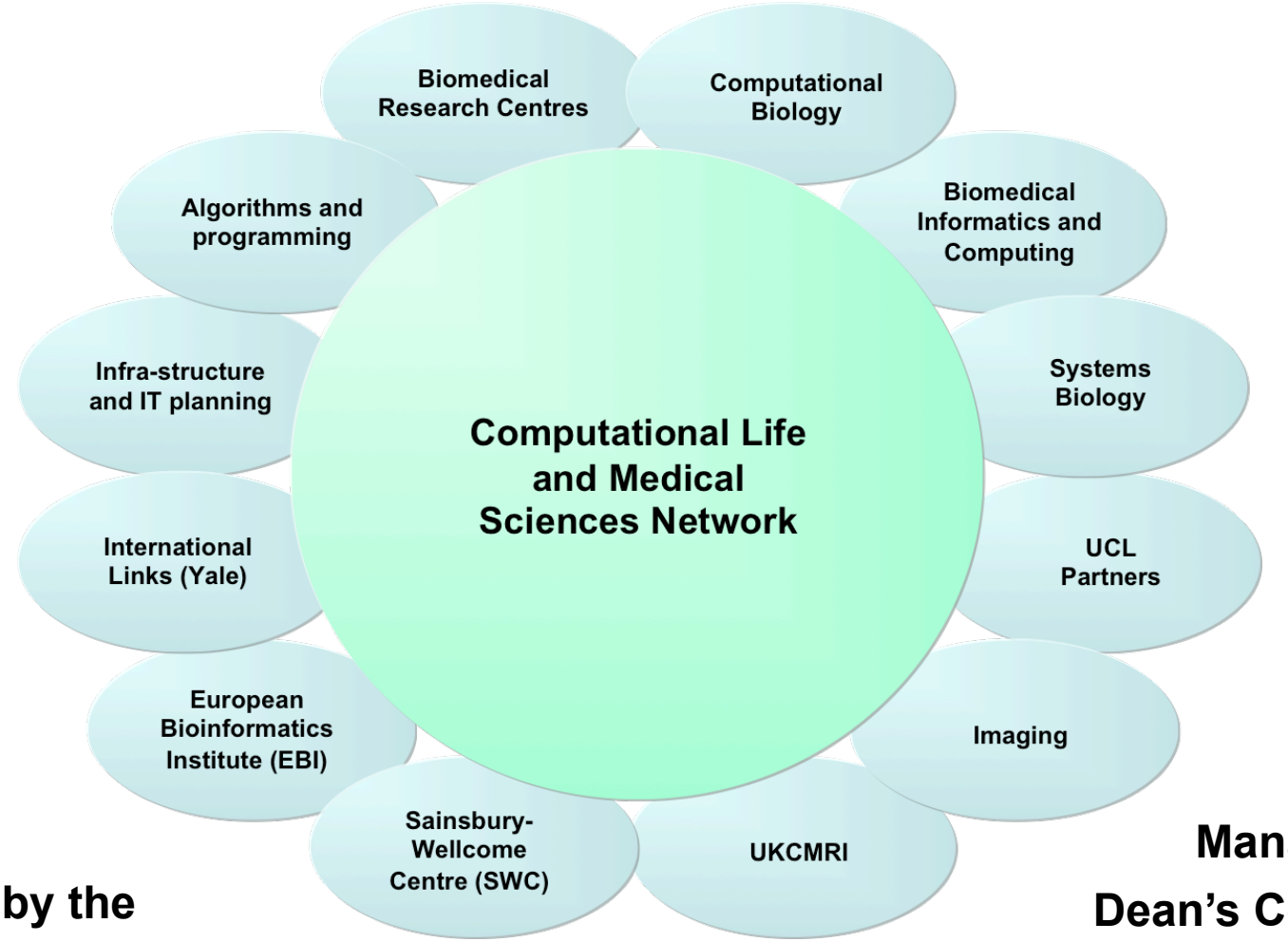
- EU FET Flagship project:
  - one of 6 pilot projects funded with €1.5M each for 12 months from May 2011
  - two pilot projects will be selected and launched as full FET Flagship initiatives in 2013
  - successful initiatives will receive €1billion over 10 years
- Led by Prof Hans Lehrach atMPI Molecular Genetics, Berlin
- UCL is a key player, leading a WP on Computing and Statistics (PI - Prof Mark Girolami)

*"ITFoM will exploit the unprecedented amounts of detailed biological data for individual people, and turn this information into actual knowledge that helps us in making medical and lifestyle decisions. By integrating the available biological data we will construct computational models of the biological processes that occur in every human. Since everybody is different, the models will be tailored to each individual to reflect their own unique anatomical, physiological and genetic makeup."*

**http://itfom.eu/**

# Computational Life and Medical Science

**The CLMS Network is 3 year initiative from September 2010**




**Supported by the Provost's Strategic Fund**

**Management:**
**Dean's Committee**
**Steering Committee**

# CLMS Goals

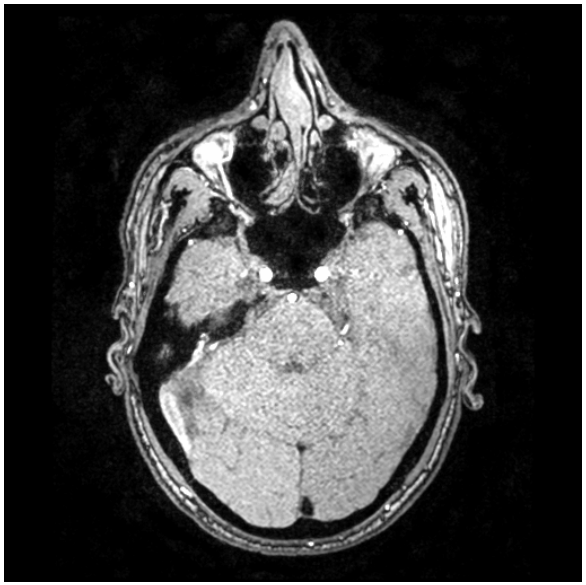
1. Maintain and expand UCL's world-leading position in life and biomedical sciences

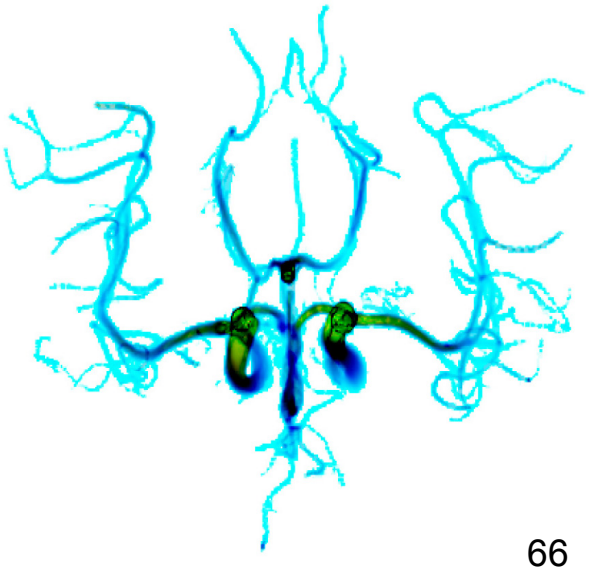
2. Improve collaboration with academic institutions: within UCL, with UCLP and the NHS, UK-CMRI, Yale, and others

3. Take advantage of new initiatives in integrative biomedical systems science from the UK Research Council, EU and others around the world

4. Improve collaboration with industry, create business and commercial opportunities, promot UCL IP licensing

5. Plan for the next stages of activity in computational life and medical sciences at UCL





# Conclusions

- The projects presented are all data intensive and all future projects will be.
  - Biomedicine community is starving for storage;
  - Network bandwidth now limiting - faster network is needed for data movement.
- Training, access and utilisation – major need:
  - Train future physicians, doctors, medics, clinicians
  - Design usable software for the above community - not only for bioinformaticians – that enable learning and knowledge extraction.
- Security and privacy
  - Need for usable mechanisms; security awareness, …

# Acknowledgements


## People

- Ali Haidar
- Stefan Zasada
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- Nour Shublaq
- Ewan Birney
- Norbert Graf
- Alfons Hoekstra
- Derek Groen
- James Suter

## Funding and Projects