# Example Applications

Grid Computing (M)

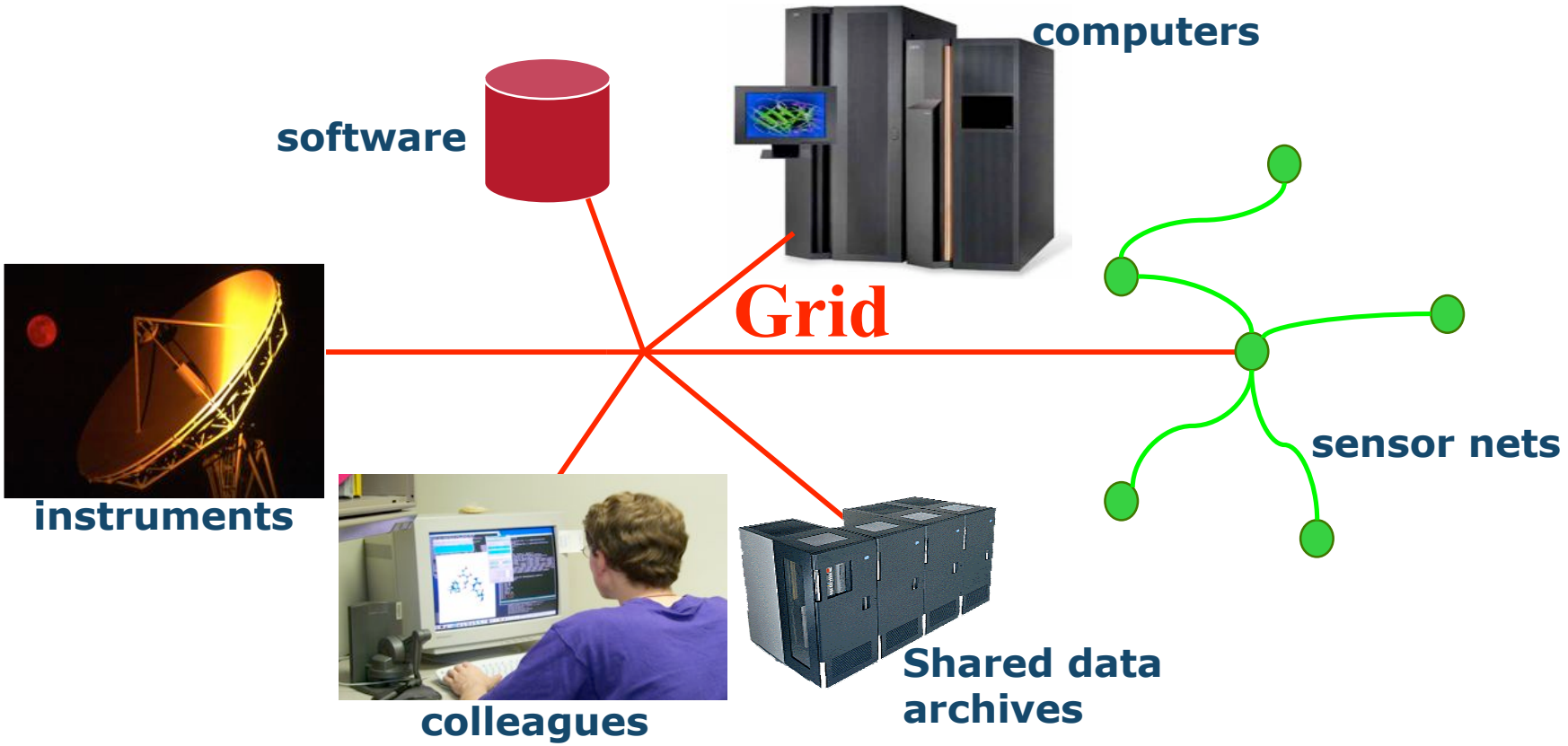
Richard Sinnott

UNIVERSITY of GLASGOW

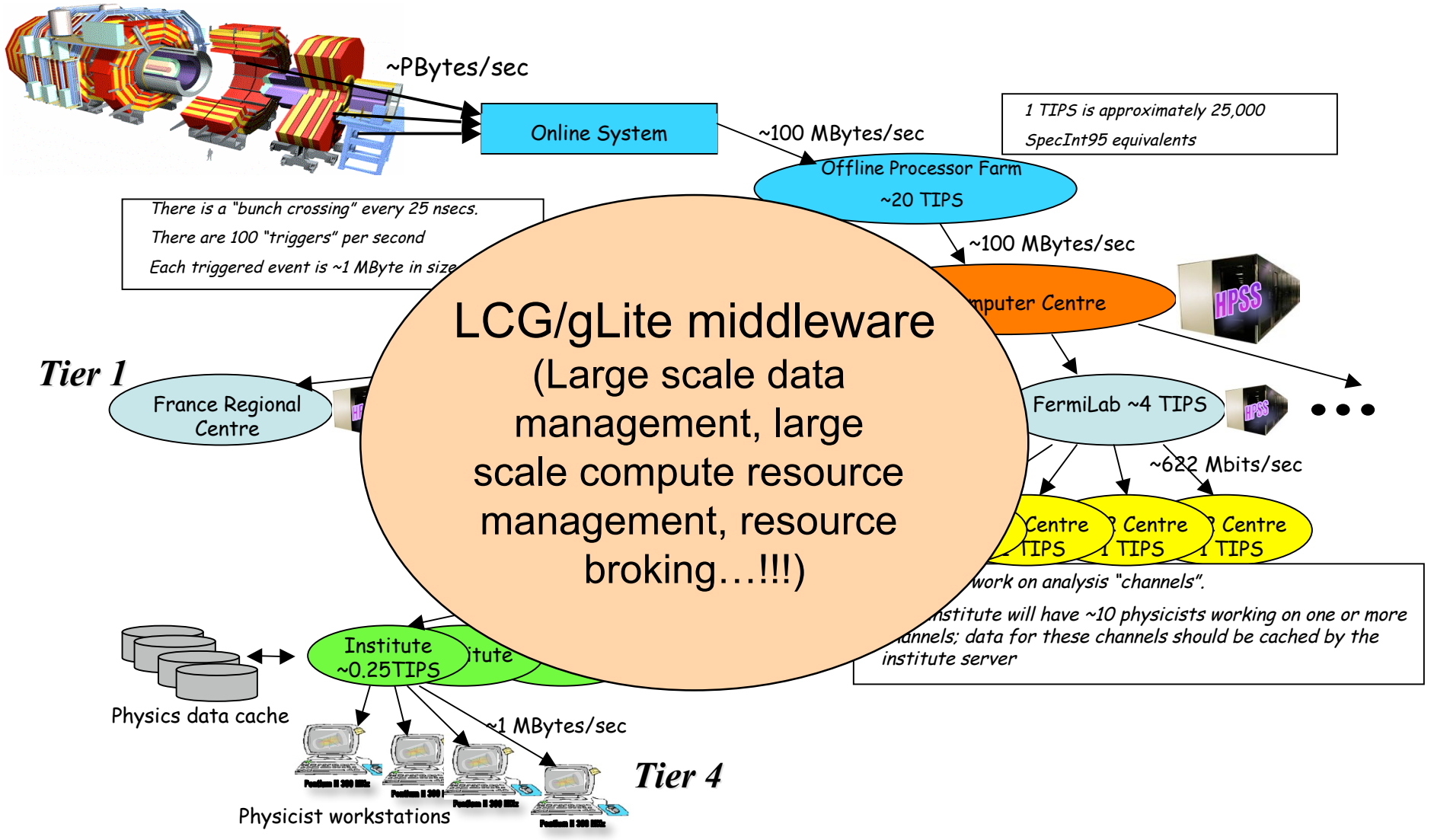


# Grid based e-Research

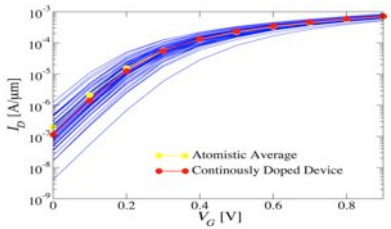
- e-Research driven by exponential growth in data, compute demands across many domains
  - Supports inter-disciplinary research
  - Enables a whole-system approach

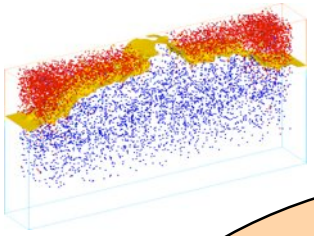


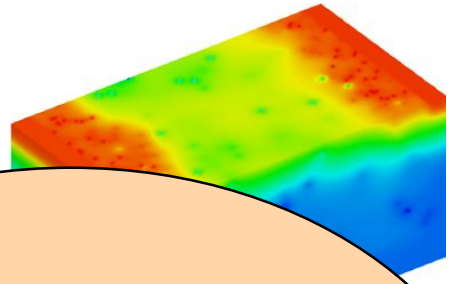
# Data Grids for High Energy Physics

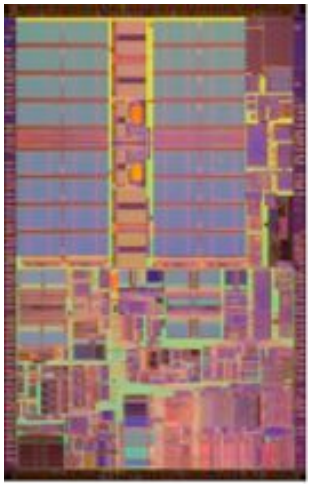


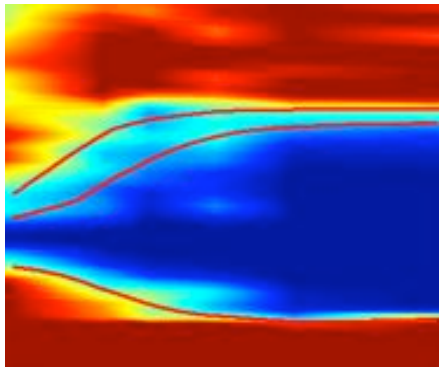
# Challenges of NanoCMOS Design



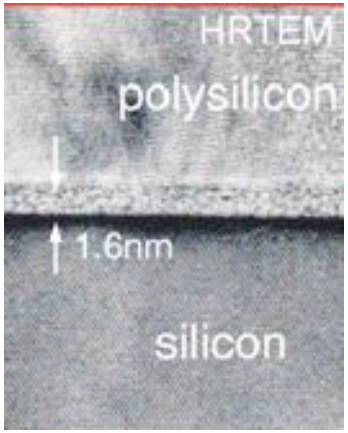



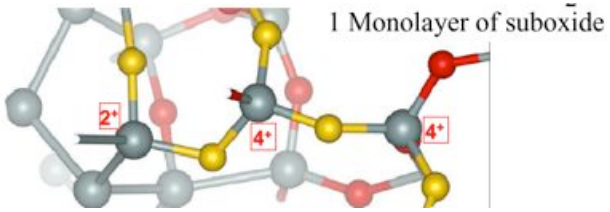


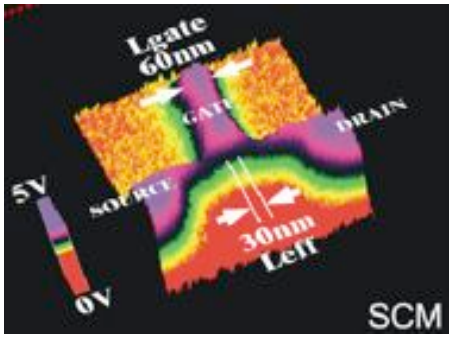




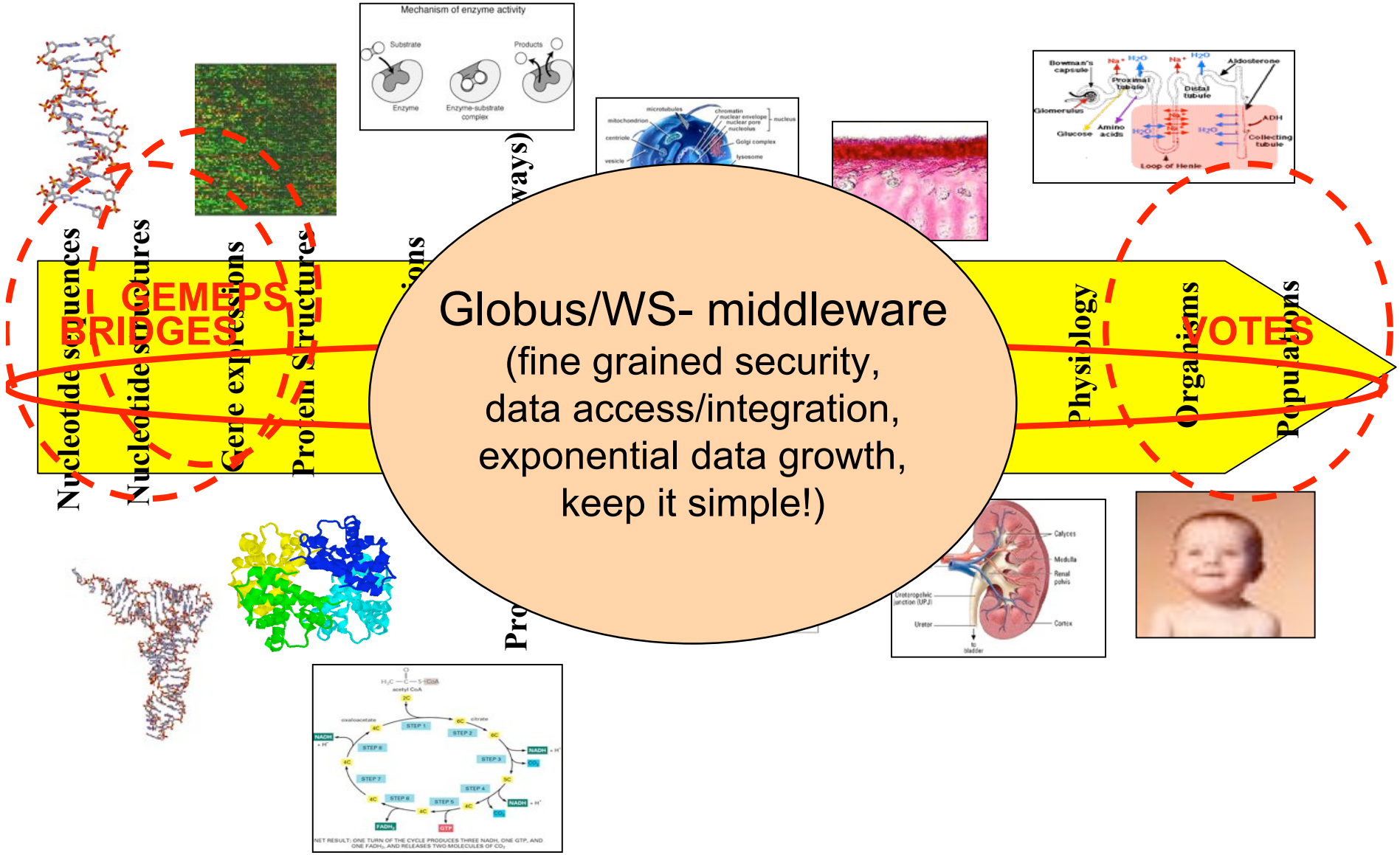
OMII-UK middleware
(workflows, security,
data management,
resource management,
…)



# The e-Health Future…

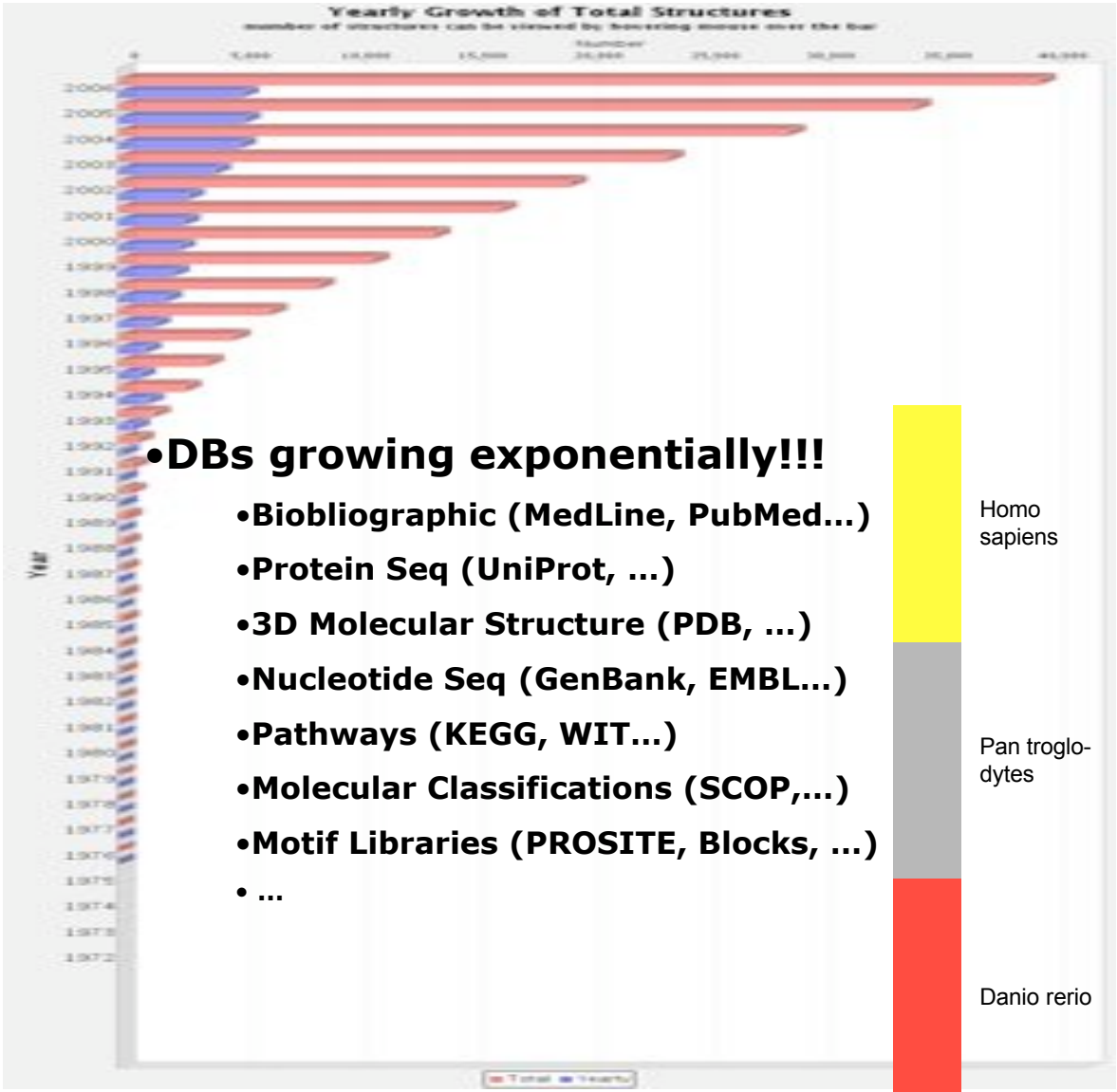


# Life Sciences

- Extensive Research Community
  - Typically more than 1000 per research university
  - Over 4500 at Glasgow University
- Many people care about them
  - Health, Food, Environment – truly interdisciplinary!
- Interacts with virtually every discipline
  - Physics, Chemistry, Maths/Stats, Nano-engineering, …
- 450+ databases relevant to bioinformatics (and growing!)
  - Heterogeneity, Interdependence, Complexity, Change, …
- Some of the Big Questions/Challenges
  - How does a cell work?
  - How does a brain work?
  - How does an organism develop?
  - Why do people who eat less tend to live longer?
  - …

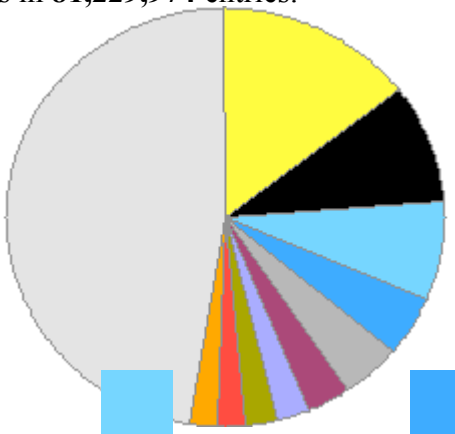
# Database Growth

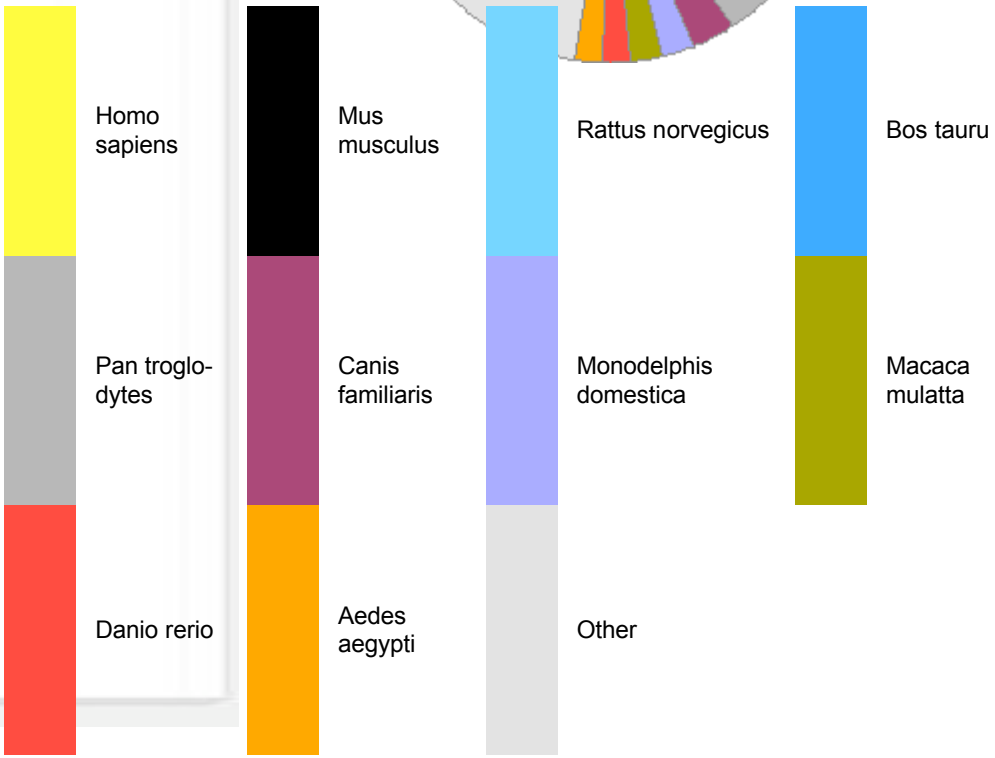
## PDB Content Growth




- **DBs growing exponentially!!!**
  - **Biobliographic (MedLine, PubMed…)**
  - **Protein Seq (UniProt, …)**
  - **3D Molecular Structure (PDB, …)**
  - **Nucleotide Seq (GenBank, EMBL…)**
  - **Pathways (KEGG, WIT…)**
  - **Molecular Classifications (SCOP,…)**
  - **Motif Libraries (PROSITE, Blocks, …)**
  - **…**

last time I checked…
EMBL Database contained **147,881,486,173** nucleotides in **81,229,974** entries.







*Yersinia pestis*



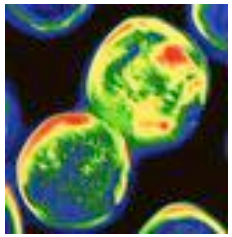
*Arabidopsis thaliana*



*Buchnerasp. APS*



*Aquifex aeolicus*



*Archaeoglobus fulgidus*



*Borrelia burgorferi*



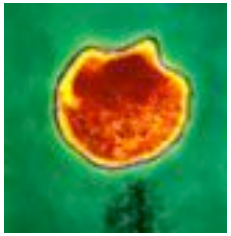
*Mycobacterium tuberculosis*



*Caenorhabitis elegans*



*Campylobacter jejuni*



*Chlamydia pneumoniae*



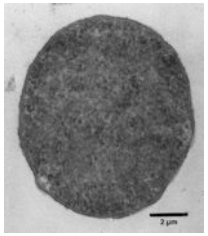
*Vibrio cholerae*



*Drosophila melanogaster*



*Escherichia coli*



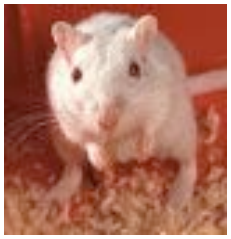
*Thermoplasma acidophilum*



*Helicobacter pylori*



*Mycobacterium leprae*



*mouse*



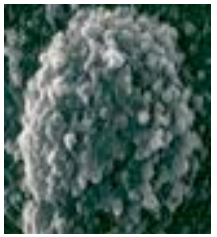
*Neisseria meningitidis Z2491*



*Plasmodium falciparum*



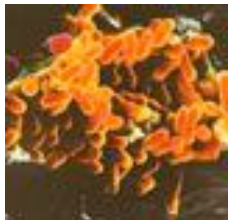
*Pseudomonas aeruginosa*



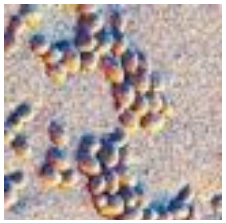
*Ureaplasma urealyticum*



*rat*



*Rickettsia prowazekii*



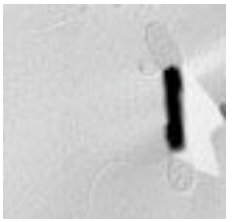
*Saccharomyces cerevisiae*



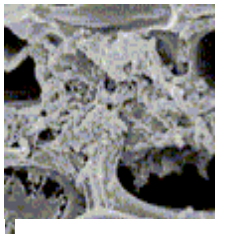
*Salmonella enterica*



*Bacillus subtilis*



*Thermotoga maritima*



*Xylella fastidiosa*

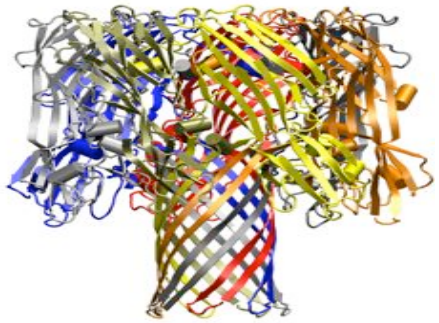
# Distributed and Heterogeneous data

## Sequence

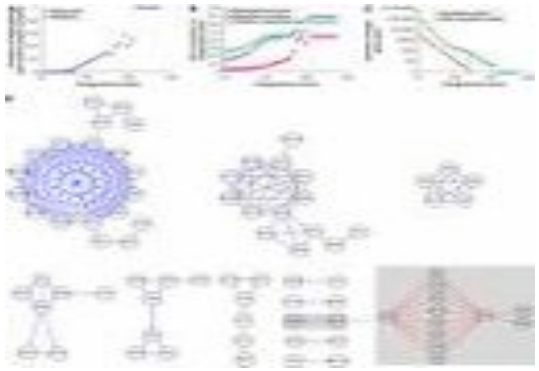
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CGCGCGCGATATATAGCGCGCG

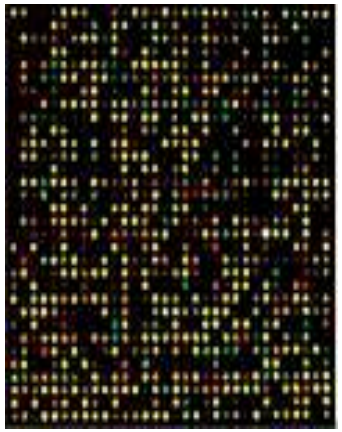
## Structure



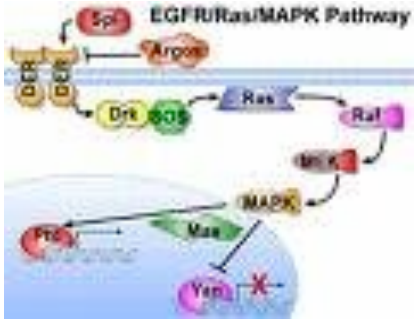
## Function



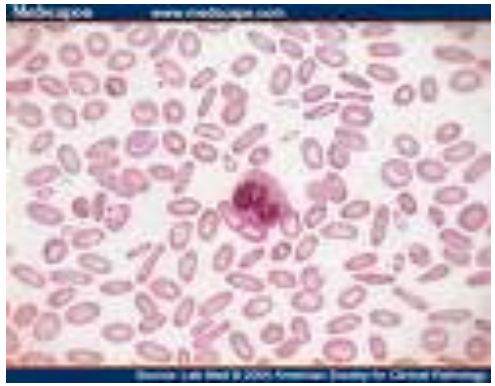
## Gene expression



## Pathways




## Morphology

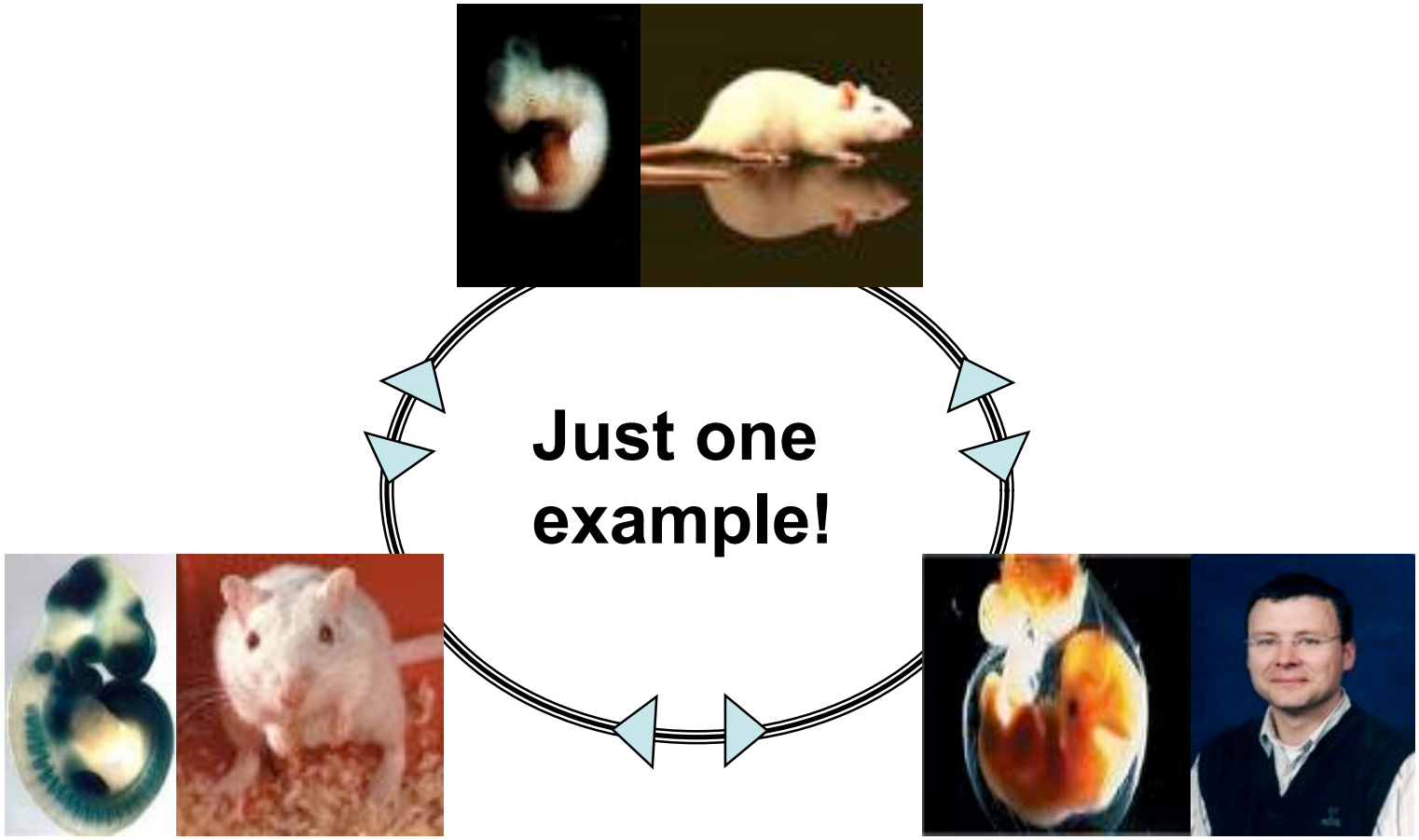


# Messy

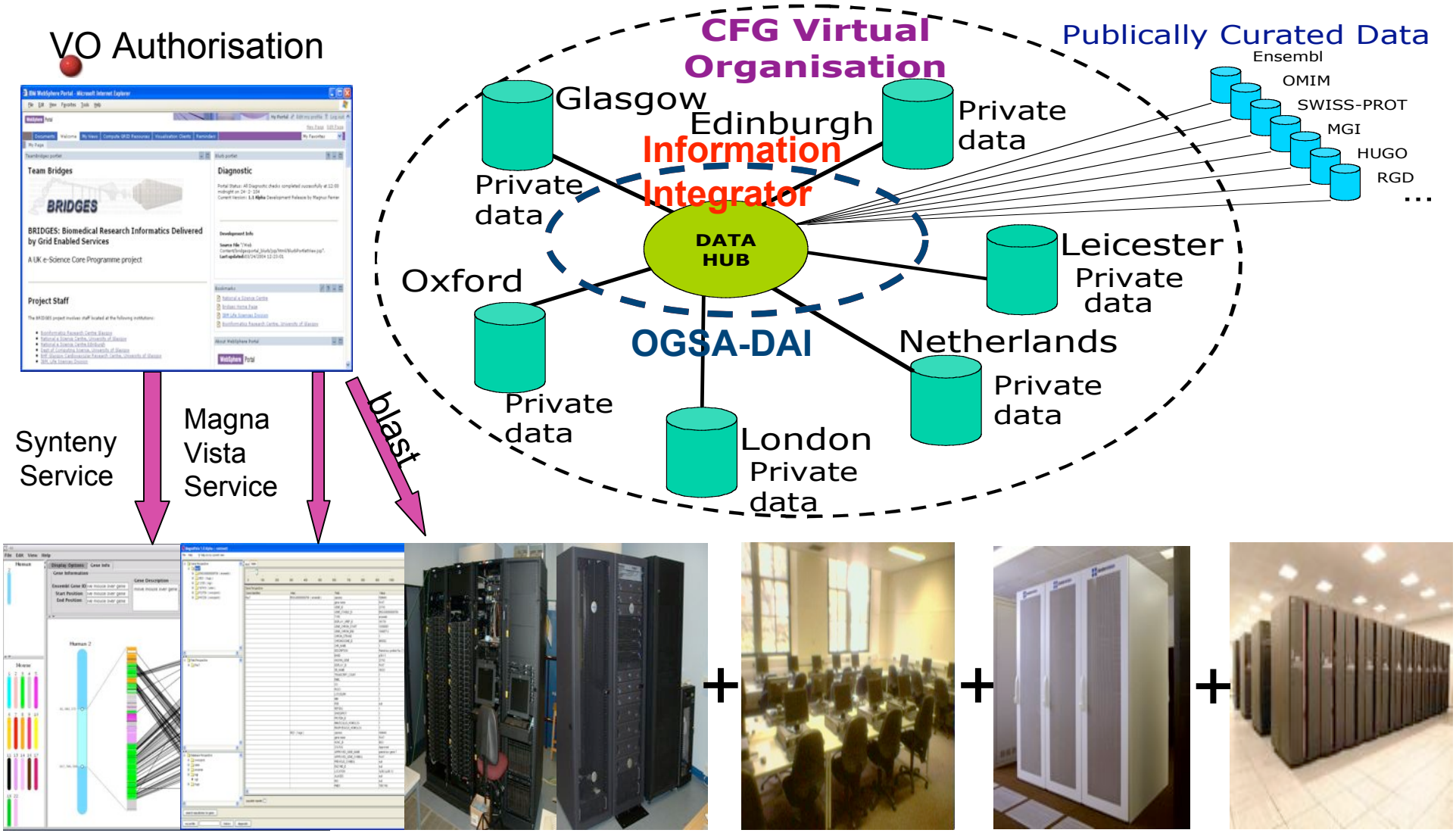



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n replication factor C, 40-kDa subunit (A1) mRNA, complete cds  1590610 M87338  RFC2                    8117_at heat shock 70kDa protein 6 (HSP
5                    8141_at       cytochrome P450, family 2, subfamily E, polypeptide 1          Human cytochrome P450IIE1 (ethanol-indu
an farnesyl-protein transferase beta-subunit mRNA, complete cds 292032  L00635  FNTB                    8177_at phospholipase D1, phosphatidylc
86096   NM_000991      RPL28                  8200004_at     eukaryotic translation initiation factor 4 gamma, 2            Homo sapiens eu
          8200010_at     ribosomal protein L11          Homo sapiens ribosomal protein L11 (RPL11), mRNA       15431289       NM_0009
_002954 RPS27A                 8200018_at     ribosomal protein S13          Homo sapiens ribosomal protein S13 (RPS13), mRNA       1459191
S5 (RPS5), mRNA 71164878       NM_001009      RPS5                   8200025_s_at    ribosomal protein L27          Homo sapiens ribosomal
(RPS11), mRNA  34335149        NM_001015      RPS11                  8200032_s_at    ribosomal protein L9           Homo sapiens ribosomal
200039_s_at    proteasome (prosome, macropain) subunit, beta type, 2          Homo sapiens proteasome (prosome, macropain) subunit, beta type
member 1             Homo sapiens ATP-binding cassette, sub-family F (GCN20), member 1 (ABCF1), transcript variant 2, mRNA   69354731
ing factor 2, 45kDa (ILF2), mRNA       24234746       NM_004515      ILF2                   8200063_at      sperm associated antigen 7
SCC3L1                 8200069_s_at    ras homolog gene family, member A          Homo sapiens ras homolog gene family, member A, mRNA (c
2268    AF275719       HSP90AB1                       8200085_s_at    ADP-ribosylation factor 1              Homo sapiens clone 24537 ADP-ri
eterogeneous nuclear ribonucleoprotein M               Homo sapiens M4 protein deletion mutant mRNA, complete cds     3126877 AF061832
RNA (cDNA clone MGC:4498 IMAGE:2964510), complete cds  33873258       BC005876       ATP6V0B                 8200079_s_at    lysyl-tRNA synt
014267  C11orf58               8200086_s_at    transcription elongation factor B (SIII), polypeptide 2 (18kDa, elongin B)
rase, CAAX box, alpha (FNTA), transcript variant 2, mRNA//Homo sapiens farnesyltransferase, CAAX box, alpha (FNTA), transcript variant 3, mRNA
omo sapiens ATPase, H+ transporting, lysosomal 9kDa, V0 subunit e (ATP6V0E), mRNA     50593534       NM_003945      ATP6V0E
U                      8200594_x_at    heterogeneous nuclear ribonucleoprotein U (scaffold attachment factor A)               Homo sapiens he
, mRNA  4507676 NM_003299      HSP90B1                8200599_s_at    heat shock protein 90kDa beta (Grp94), member 1        Homo sapiens he
ein kinase, CAMP-dependent, regulatory, type I, alpha (tissue specific extinguisher 1) (PRKAR1A), transcript variant 3, mRNA    47132579///4713
006265  RAD21                  8200609_s_at    WD repeat domain 1             Homo sapiens WD repeat domain 1 (WDR1), transcript variant 1, m
rotein complex 2, beta 1 subunit (AP2B1), transcript variant 2, mRNA    71773105///71773037    NM_001030006///NM_001282       AP2B1
n 3 (phosphorylase kinase, delta)      Homo sapiens calmodulin 3 (phosphorylase kinase, delta) (CALM3), mRNA   58218967       NM_0051
mRNA    47419917       NM_004184      WARS                   8200630_x_at    SET translocation (myeloid leukemia-associated)        Homo sa
Homo sapiens protein tyrosine phosphatase, receptor type, F (PTPRF), transcript variant 1, mRNA 109633040      NM_002840      PTPRF
ystophan 5-monooxygenase activation protein, zeta polypeptide          Homo sapiens tyrosine 3-monooxygenase/tryptophan 5-monooxygenase activa
0646_s_at      nucleobindin 1          Homo sapiens nucleobindin 1 (NUCB1), mRNA      39725676       NM_006184      NUCB1
d protein beta)        Homo sapiens signal sequence receptor, beta (translocon-associated protein beta) (SSR2), mRNA   4552341 NM_003145
ide translocator), member 6 (SLC25A6), mRNA    4502098 NM_001152      SLC25A5                8200658_s_at    prohibitin             Homo sa
NM_006145      DNAJB1                 8200665_s_at    secreted protein, acidic, cysteine-rich (osteonectin)          Homo sapiens secreted p
g protein 1 (XBP1), mRNA       14110394       NM_005080      XBP1                   8200671_s_at    spectrin, beta, non-erythrocytic 1
7977    NM_003347      UBE2L3                 8200677_at      pituitary tumor-transforming 1 interacting protein             Homo sapiens pi
nt 1, mRNA//Homo sapiens ubiquitin-conjugating enzyme E2L 3 (UBE2L3), transcript variant 2, mRNA       38157977///38157975    NM_003347///NM_
on factor 1 gamma              Homo sapiens eukaryotic translation elongation factor 1 gamma (EEF1G), mRNA    83656774       NM_001404
D (Asp-Glu-Ala-Asp) box polypeptide 24 (DDX24), mRNA   14251213       NM_020414      DDX24                  8200695_at      protein phospha
mRNA    8051609 NM_006854      KDELR2                 8200700_s_at    KDEL (Lys-Asp-Glu-Leu) endoplasmic reticulum protein retention receptor
6127    NM_001959      EEF1B2                 8200706_s_at    lipopolysaccharide-induced TNF factor          Homo sapiens lipopolysaccharide
bule-associated protein, RP/EB family, member 1        Homo sapiens microtubule-associated protein, RP/EB family, member 1 (MAPRE1), mRNA
phase kinase-associated protein 1A (p19A) (SKP1A), transcript variant 2, mRNA   25777710///25777712    NM_006930///NM_170679   SKP1A
t 2, mRNA      61676201///61676202    NM_005898///NM_203364   GPIAP1                 8200723_s_at    GPI-anchored membrane protein 1
apiens ARP2 actin-related protein 2 homolog (yeast) (ACTR2), transcript variant 1, mRNA///Homo sapiens ARP2 actin-related protein 2 homolog (ye
AX1 (RPTPCAAX1) mRNA, complete cds     1777754 U48296  PTP4A1                  8200734_s_at    ADP-ribosylation factor 3              Homo sa
3 (S. cerevisiae) (SUMO3), mRNA 48928057       NM_006936      SUMO3                  8200741_s_at    ribosomal protein S27 (metallopanstimul
6       NM_002074      GNB1                   8200747_s_at    nuclear mitotic apparatus protein 1            Homo sapiens nuclear mitotic ap
e/serine-rich 2        Homo sapiens splicing factor, arginine/serine-rich 2 (SFRS2), mRNA     47271442       NM_003016      SFRS2
P-ribosylation-like factor 6 interacting protein 5             Homo sapiens ADP-ribosylation-like factor 6 interacting protein 5 (ARL6IP5), mR
nce similarity 120A (FAM120A), mRNA    68299753       NM_014612      FAM120A                8200768_s_at    methionine adenosyltransferase
rity 120A (FAM120A), mRNA      68299753       NM_014612      FAM120A                8200775_s_at    heterogeneous nuclear ribonucleoprotein
491///NM_001008492///NM_004404///NM_006155     SEPT2                  8200779_at      activating transcription factor 4 (tax-responsive enhan
n-related protein 1 (alpha-2-macroglobulin receptor)           Homo sapiens low density lipoprotein-related protein 1 (alpha-2-macroglobulin r
sapiens IQ motif containing GTPase activating protein 1 (IQGAP1), mRNA  57242794       NM_003870      IQGAP1                 8200792_at
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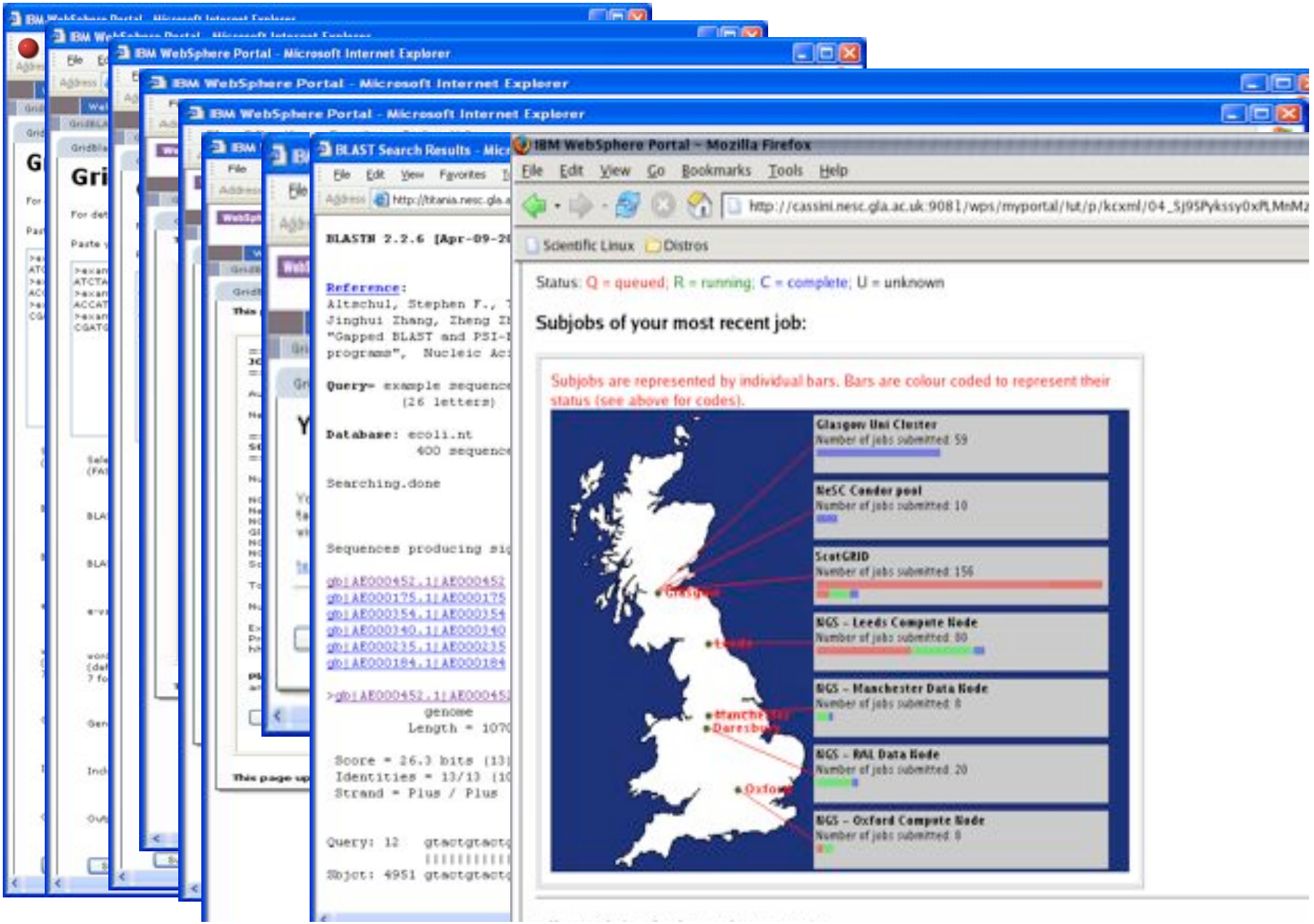
# Translational Research



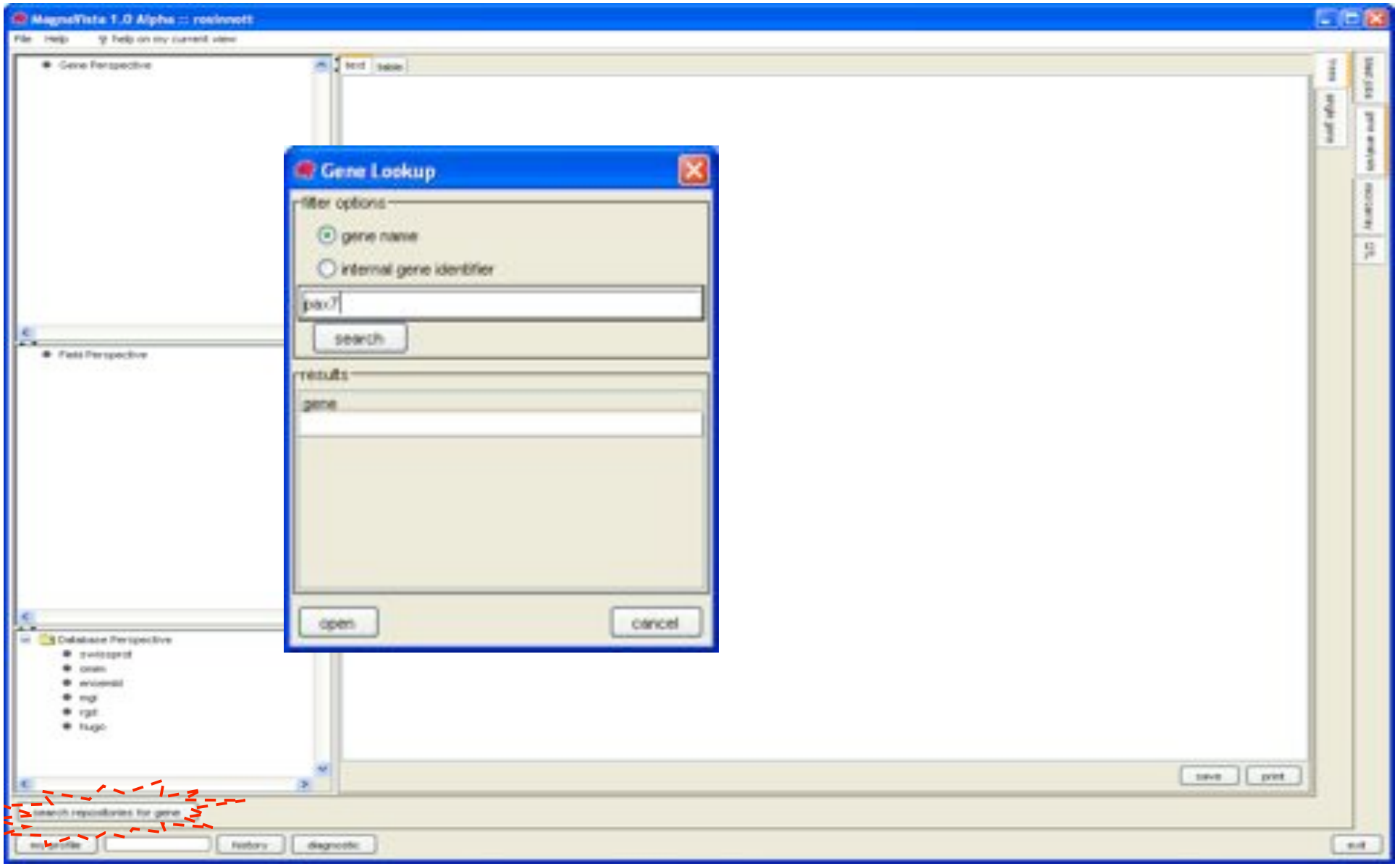
# BRIDGES Project



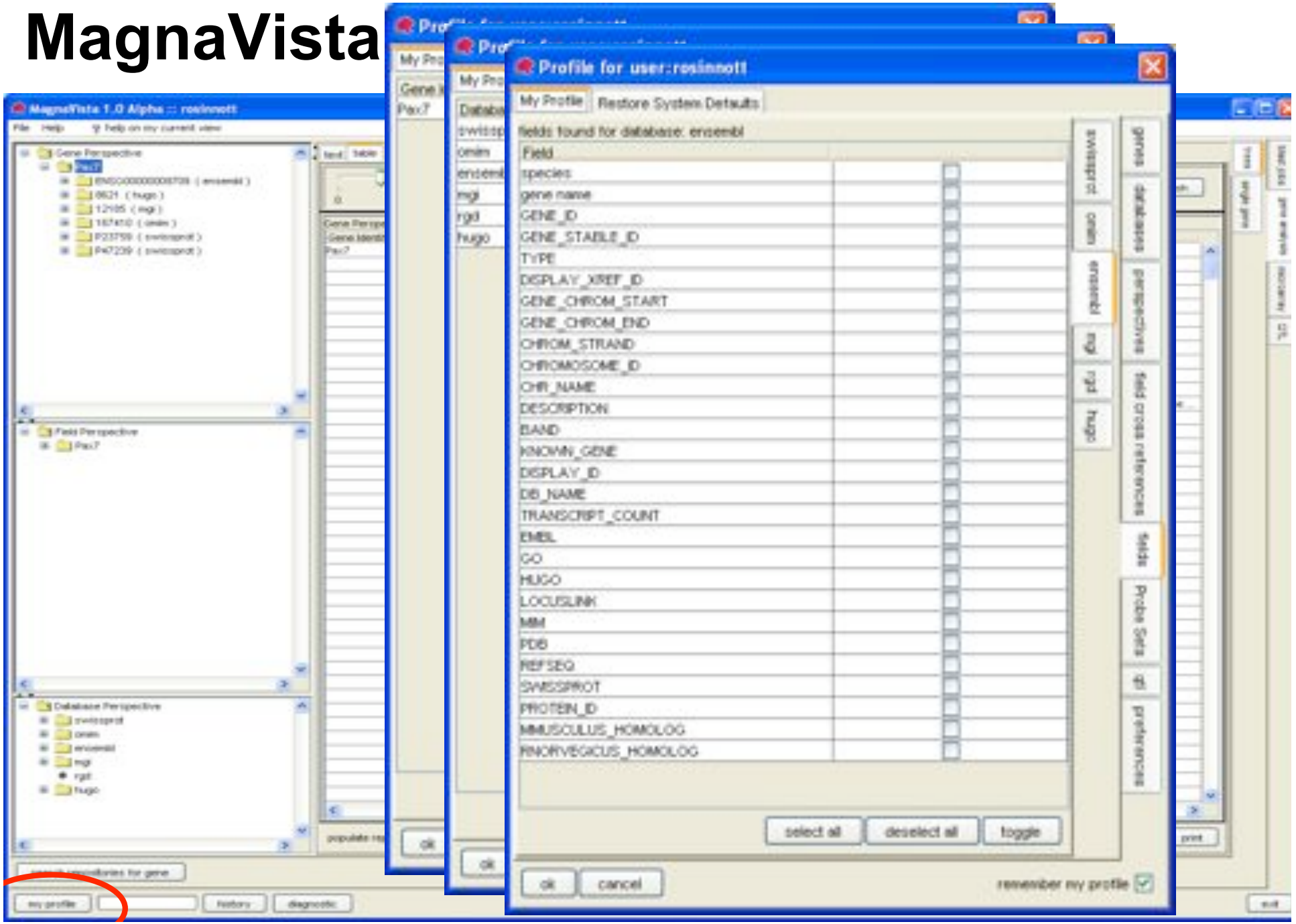
# Grid Blast Interface



# MagnaVista


Gene Lookup
filter options
gene name
internal gene identifier
search
results
gene
open
cancel

# MagnaVista


Profile for user:rosinnott
My Profile
Restore System Defaults
fields found for database: ensembl
Field
species
gene name
GENE_ID
GENE_STABLE_ID
TYPE
DISPLAY_XREF_ID
GENE_CHROM_START
GENE_CHROM_END
CHROM_STRAND
CHROMOSOME_ID
CHR_NAME
DESCRIPTION
BAND
KNOWN_GENE
DISPLAY_ID
DB_NAME
TRANSCRIPT_COUNT
EMBL
GO
HUGO
LOCUSLINK
MIM
PDB
REFSEQ
SWISSPROT
PROTEIN_ID
MMUSCULUS_HOMOLOG
RNORVEGICUS_HOMOLOG
select all
deselect all
toggle
ok
cancel
remember my profile
swissprot
omim
ensembl
mgi
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fields
Probe Sets
qtl
preferences

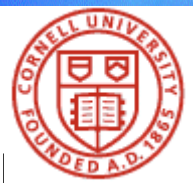
# GeneVista


IBM WebSphere Portal - Microsoft Internet Explorer
File Edit View Favorites Tools Help
GeneVista
Back
GeneVista
Enter new gene name
Submit
Previous genes
PAX7
Submit
Entry Information
Entry Name PAX7_MOUSE
Primary Accession Number P47239
Date entered in SwissProt 1996-02-01
Sequence last modified 1996-02-01
Annotations last modified 2003-02-28
Name and origin of the protein
Protein name Paired box protein Pax-7
GeneName PAX7
PAX-7
From Mus musculus (Mouse) [TaxID: 10090]
Taxonomy Eukaryota ; Metazoa ; Chordata ; Craniata ; Vertebrata ; Euteleostomi ; Mammalia ; Eutheria ; Rodentia ; Sciurognathi ; Muridae ; Murinae ; Mus
References
Reference Number 0
Reference journal article
Strain -
Title The murine paired box gene, Pax7, is expressed specifically during the development of the nervous and muscular system.
Authors Jostes B. , Walther C. , Gruss P.
Appeared in Mech. Dev.
Volume 33
Pages 27 - 37
Date 1990
Tissue -
Comments
Function Probable transcription factor. May have a role in myogenesis
By similarity -
subunit Can bind to DNA as a heterodimer with PAX3. Interacts with DAXX
subcellular location Nuclear

# Grid Enabled Microarray Expression Profile Search (GEMEPS) Project

- 1 year BBSRC funded project started March 2006
  - Involves Glasgow, Cornell University, US, Riken Institute, Japan
    - 1RA at NeSC
  - Aim to provide tools for discovery, comparison a analysis of microarray data sets




- BRIDGES focused on genes of interest
- GEMEPS focuses on microarrays consisting of many thousands of genes of interest
  - Gene expression profiles

# Key Scenarios

- **Key questions to be answered by GEMEPS infrastructure:**
  - who has run a microarray experiment and generated *similar* results to mine?
    - How similar were these results?
  - who has undertaken experiments and produced data relevant to my own interests,
    - for a particular phenotype,
    - for a particular cell type,
    - for a particular pathogen,
    - on a particular platform
    - …
  - show me the conditions and analysis associated with experimental results similar to mine
  - …

# Microarray Repositories and Data Formats

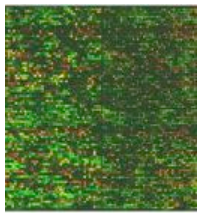
- MIAME goal is
  - *minimum information required to interpret unambiguously and potentially reproduce and verify an array based gene expression monitoring experiment*
- Several data formats/controlled vocabularies and ontologies defined and applied across different sites communities including
  - MAGE-ML - Microarray Gene Expression Markup Language
  - SOFTtext – Simple Omnibus Format in Text
  - MINiML – MIAME Notation in Markup Language
  - SOFTmatrix - Simple Omnibus Format in Matrix
  - …
- Main repositories explored include
  - Gene Expression Omnibus (GEO),
  - ArrayExpress,
  - CIBEX

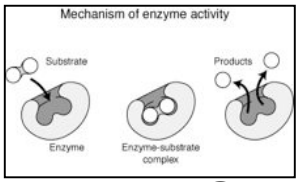
# GEMEPS Discovery and Analysis of Matching Profiles

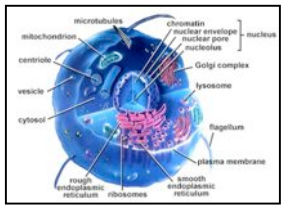
- **Step 1:**
  - **Query over appropriate meta-data and return matching experiments**
    - (appropriate to level of privilege)
- **Step 2:**
  - **For matching results**
    - extract gene ordering (based on level of expression values)
      - Can include filtering/cut off, e.g. so only compare only 10, 100, 1000, … most expressed genes from experiments
    - run similarity algorithm to determine best match of own data results against experiment gene expression ordering
      - currently support Spearman Rank but Kendall Tau coming
- **Step 3:**
  - **Merge the results and display**

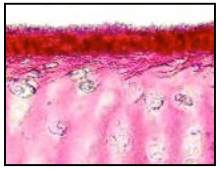
# The e-Health Future…

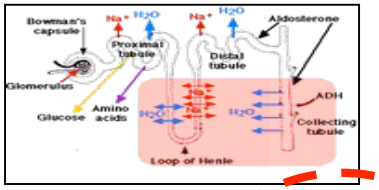











Nucleotide sequences

Nucleotide structures

Gene expressions

Protein Structures

Protein functions

Protein-protein interaction (pathways)

Cell

Cell signalling

Tissues

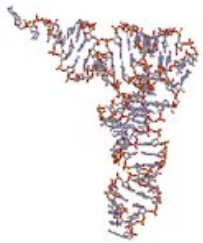
Organs

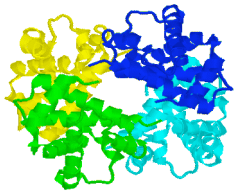
Physiology

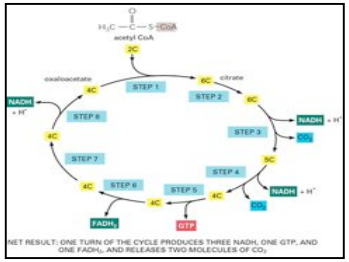
Organisms

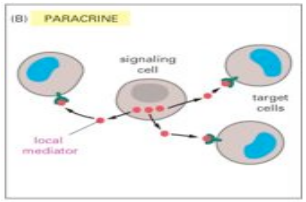
VOTES

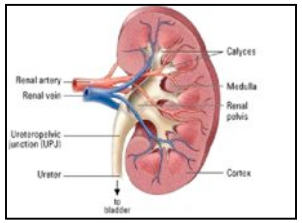
Populations







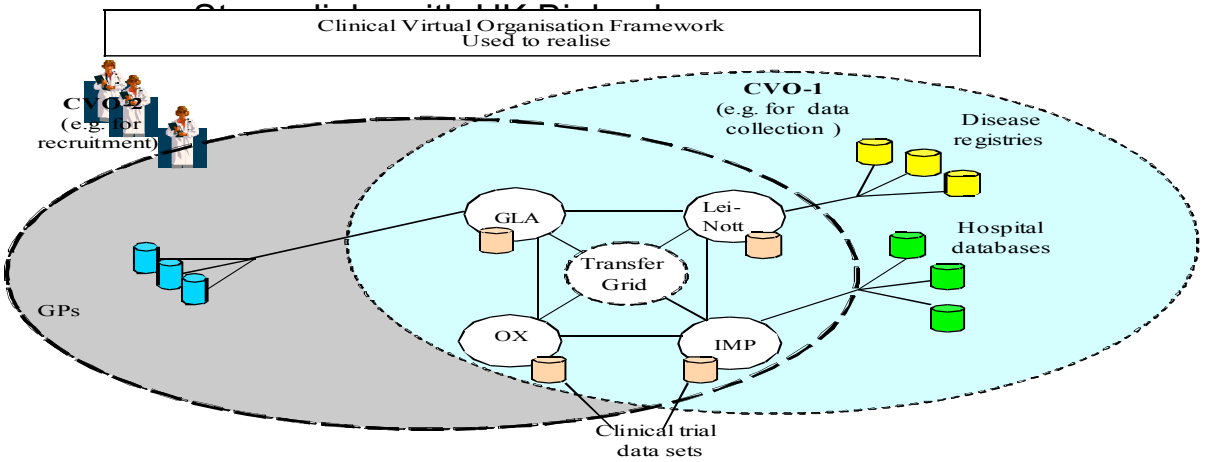





# VOTES

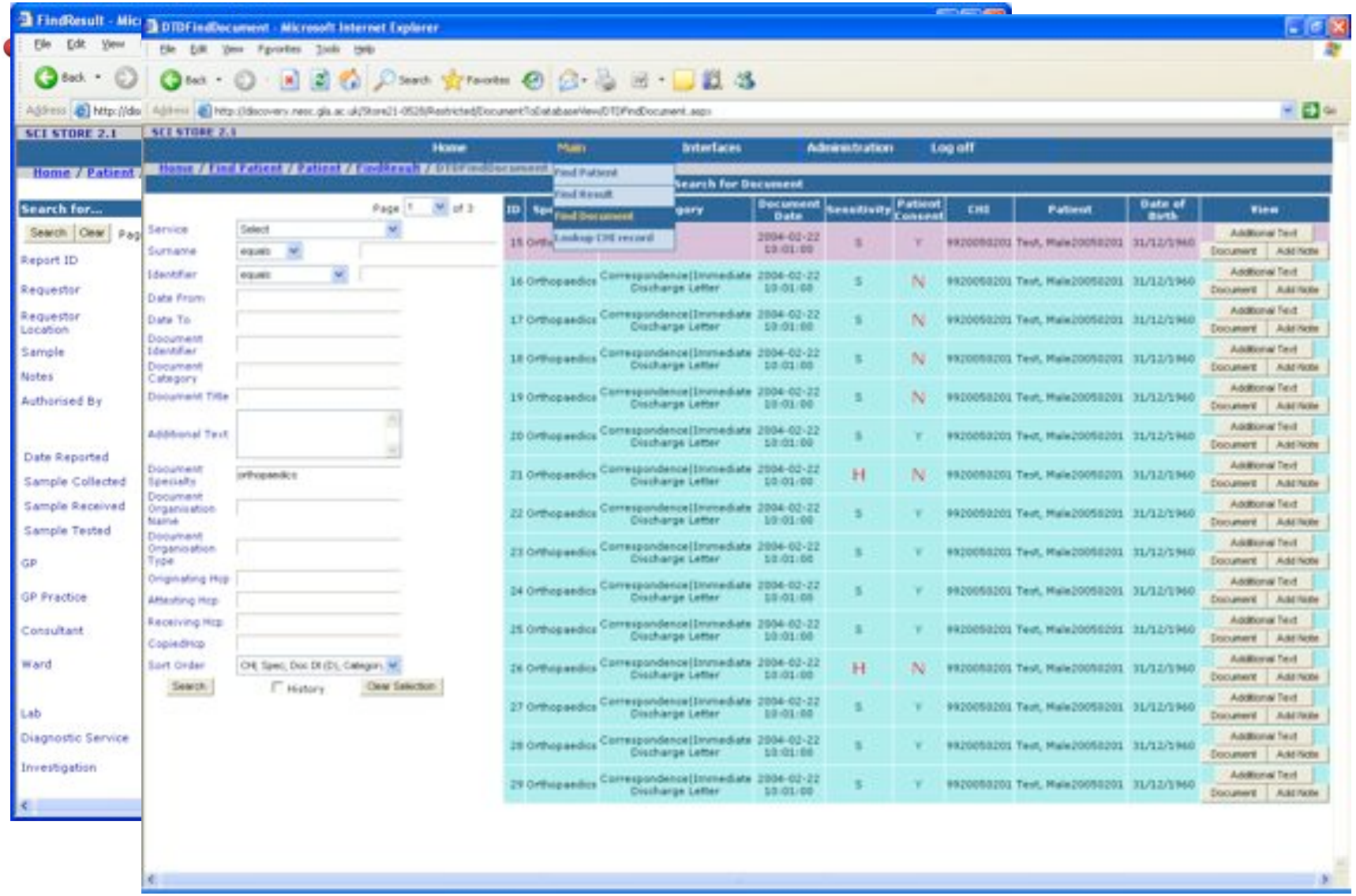
- **Virtual Organisations for Trials and Epidemiological Studies**
  - **3 year (£2.8M) MRC funded project started October 2005**
  - **Plans to develop *framework for producing Grid infrastructures* to address key components of clinical trial/observational study**
    - Recruitment of potentially eligible participants
    - Data collection during the study
    - Study administration and coordination
      - Involves Glasgow, Oxford, Leicester/Nottingham, Manchester, Imperial



# Initial Experiences

- Scottish Data Space… up to now
  - Scottish Care Information (SCI) Store
  - Scottish Morbidity Records (SMR)
  - General Practitioners Administration System for Scotland (GPASS)
  - Data dictionary
  - …
  - Consent database

# A Quick Tour of SCI Store

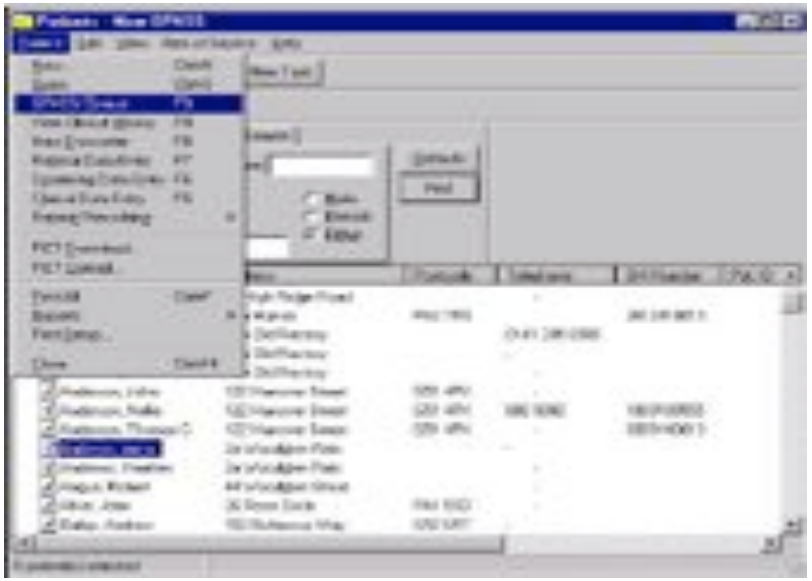


# Scottish Morbidity Records

- **Scottish Morbidity Records**
  - **Good quality data sets put together by ISD**
    - Historic SMR1 Discharges January 1981 - March 1997
    - COPPISH SMR01 Discharges April 1997 onwards
    - Historic SMR4 Discharges 1981 – March 1997
    - COPPISH SMR04 Admissions April 1996 onwards
    - GRO Death Records  January 1980 - December1995
    - GRO Death Records  January 1996 onwards
    - SOCRATES (Cancer Registrations) 1980 onwards
  - **Negotiating access to anonymised SMR data sets**

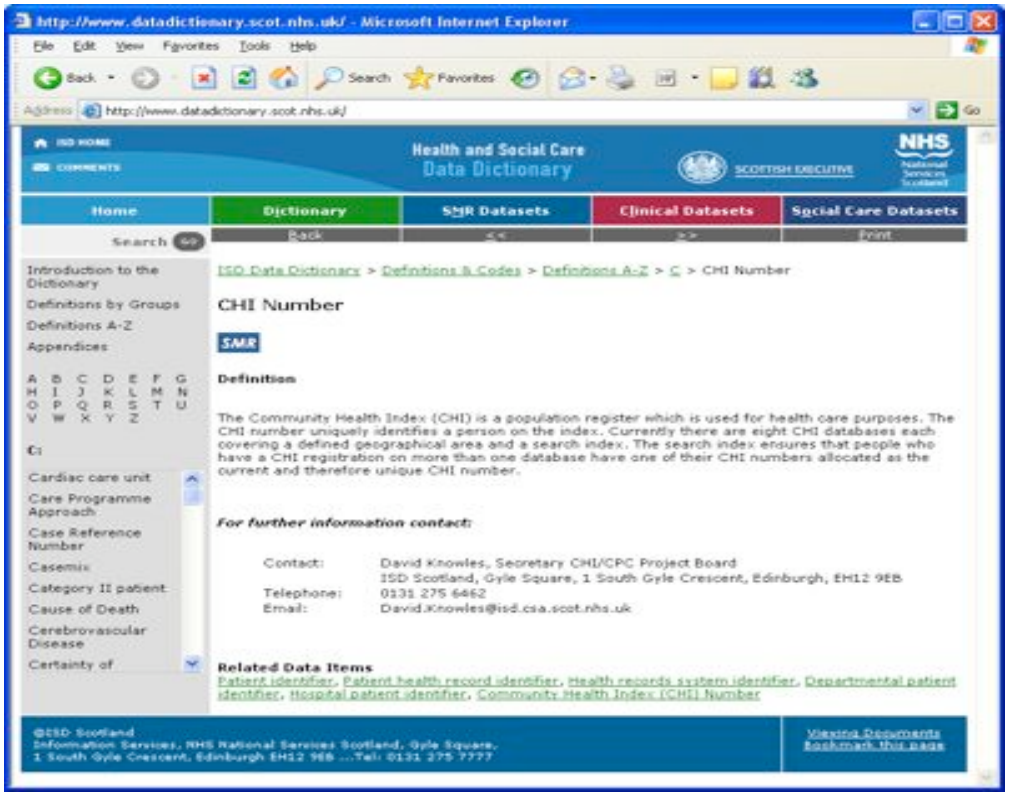
# GPASS

- **General Practice Administration System for Scotland (GPASS)**
  - **used by over 85% of GPs in Scotland**
    - links from SCI Store to GPASS
  - **access to GPASS software with training data sets**
    - XML API available for querying
      - www.gpass.co.uk



# Data Dictionary

- **Includes vocabulary for**
  - **SMR data**
  - **Clinical data**
  - **Social care data**



# Data Consent

- **Simple solution implemented at NeSC for now**
  - **E-Health strategy states it will eventually be included as part of patient electronic health record in Scotland**
- **Scenarios based upon patient consent**
  - **For general use of data**
  - **For usage of data in particular trial**
  - **For usage of data in particular disease research**
    - Combinations of these possible/likely!
  - **Opt in vs Opt out?**
    - We have implemented various scenarios to show how it might work, but need to be aligned with “real world”
      - i.e. with NHS plans/strategy for e-Health

# Prelude to Walk Through of Demo

# Security & Usability

- Grid Security
  - AAAA
- Users like usernames/passwords
  - Provide them (once!)
- Users don't like/understand X.509 based PKI
  - **Forget training, education for most users!**
    - ***$> openssl pkcs12 -in cert.p12 -clcerts -nokeys -out usercert.pem!***
  - **The vast majority most certainly won't jump through hoops to get on the Grid**
    - "me-Science" culture

# “A”AAA

- **Identity management issues**
  - **Certificate Revocation Lists**
    - When revoked? By whom? How timely?
- **Strong passwords for private keys**
  - **Users write them down, share them, forget them**
- **Privilege Management**
  - **Numerous domains where never get access to local account to “do stuff”**
    - I need to access your NHS DB to run queries, change tables, run arbitrary code…
  - **At NeSC Glasgow we have focused on**
    - improving AAAA and AAAA

# Improving "A"AAA

- **Best to exploit local authentication**
  - **Sites know best if users still at institution and are best placed to state what their privileges are/should be**
- **Introducing Shibboleth**

# Introducing Shibboleth

- **Shibboleth (http://shibboleth.internet2.edu)**

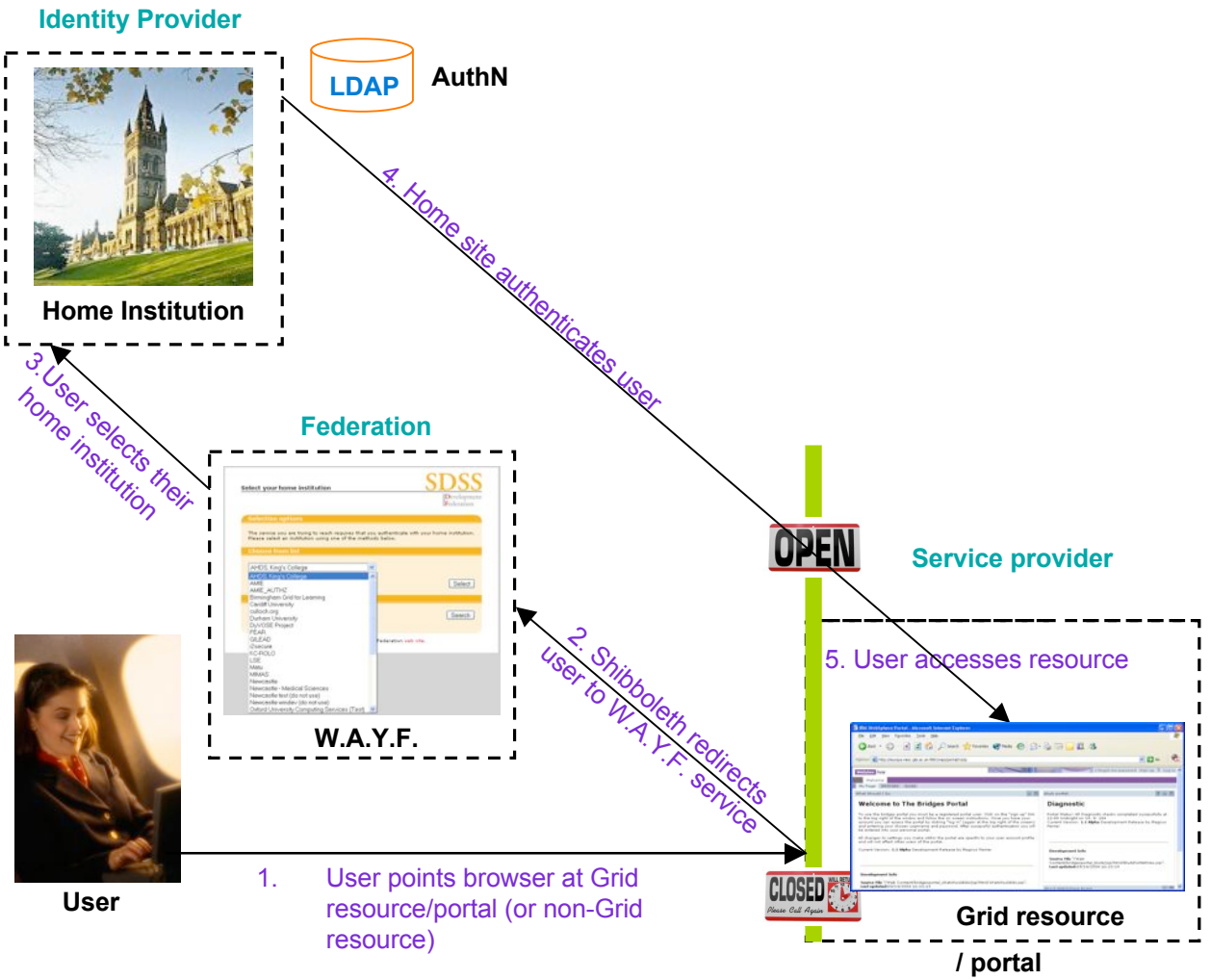
  **Definition**

  Shibboleth [Hebrew for an ear of corn, or a stream or flood]

  1. A word which was made the criterion by which to distinguish the *Ephraimites* from the *Gileadites*. The *Ephraimites*, not being able to pronounce sh, called the word sibboleth. See --Judges xii.
  2. Hence, the criterion, test, or watchword of a party; a party cry or pet phrase. ]

  - Shibboleth replacing Athens as access mgt system across UK academia
    - i.e. this is main stream and not (weird) Grid solutions!
- **Federations based on trust**
  - or more accurately trust but verify
  - numerous international federations exist MAMS, SWITCH, HAKA, SDSS…

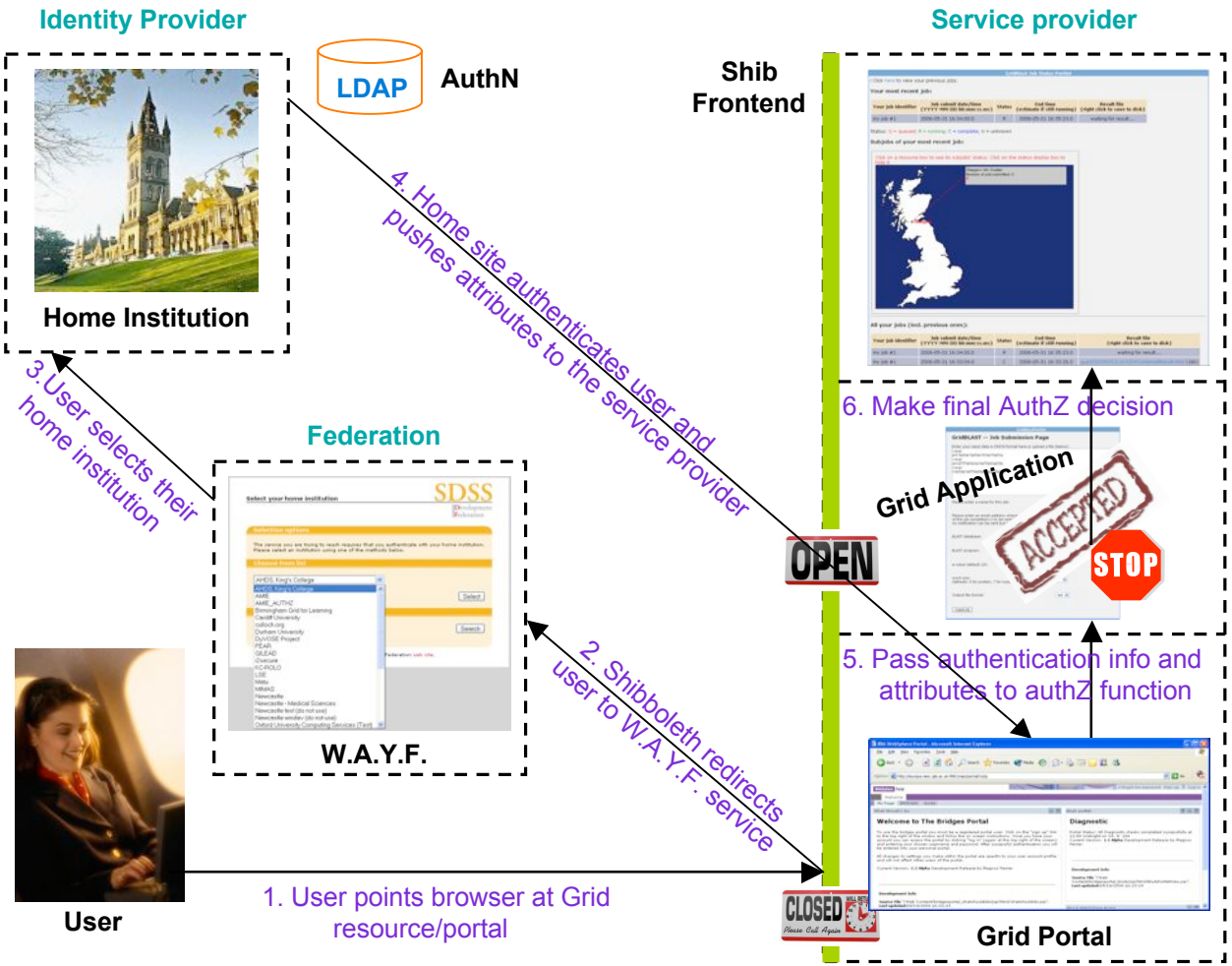
# Typical Shibboleth Scenario



# It's a start, but…

- **Benefit from local authentication but really want finer grained control…**
  - **I know you have authenticated, but I need to know that you have sufficient/correct privileges to access my VO resources**
  - **can also return various other information needed to support *authorisation* decisions**
    - At NeSC we have been working extensively with PERMIS and portal content configuration

# Finer Grained Shibboleth Scenario

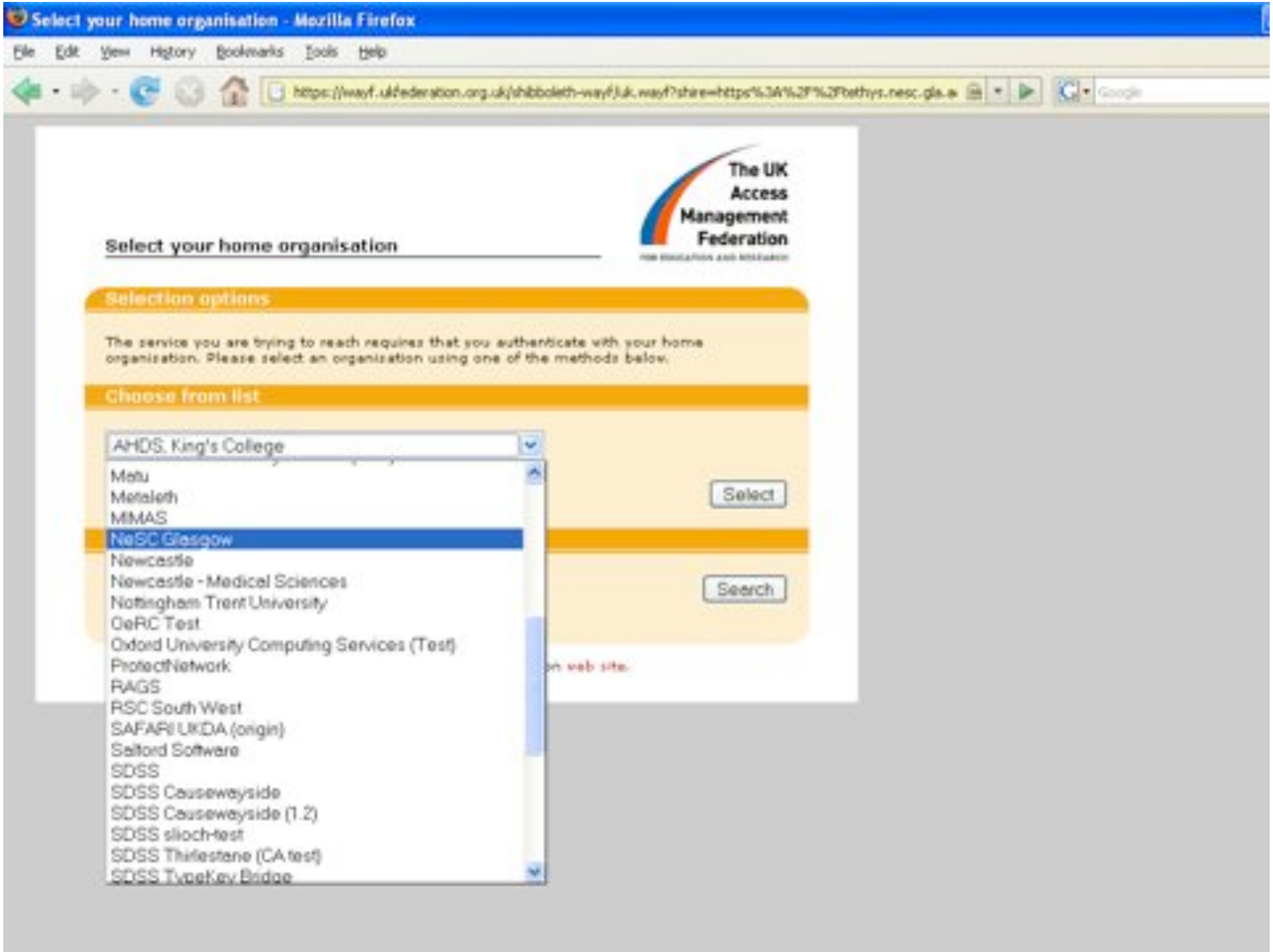


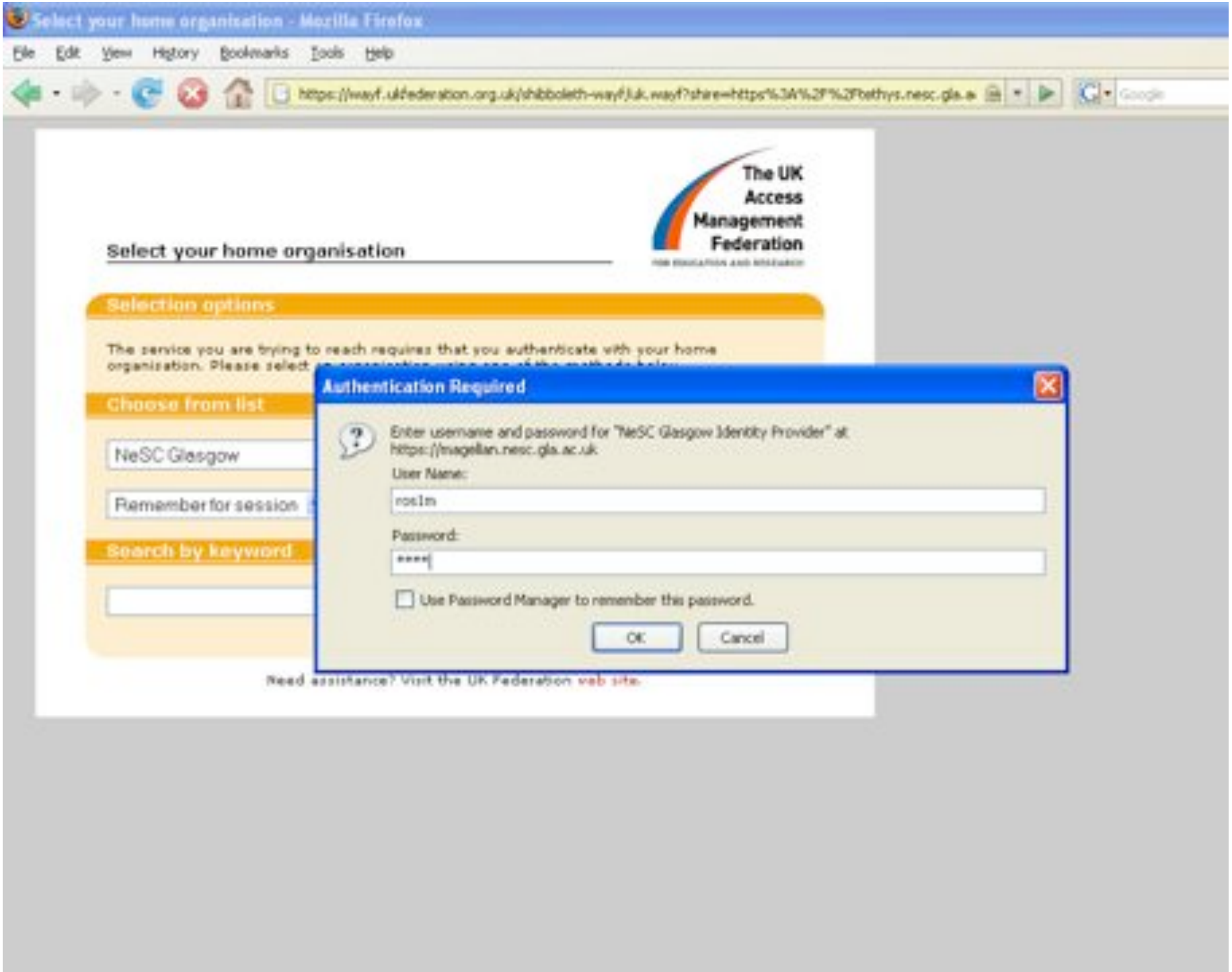
# Ok, but…

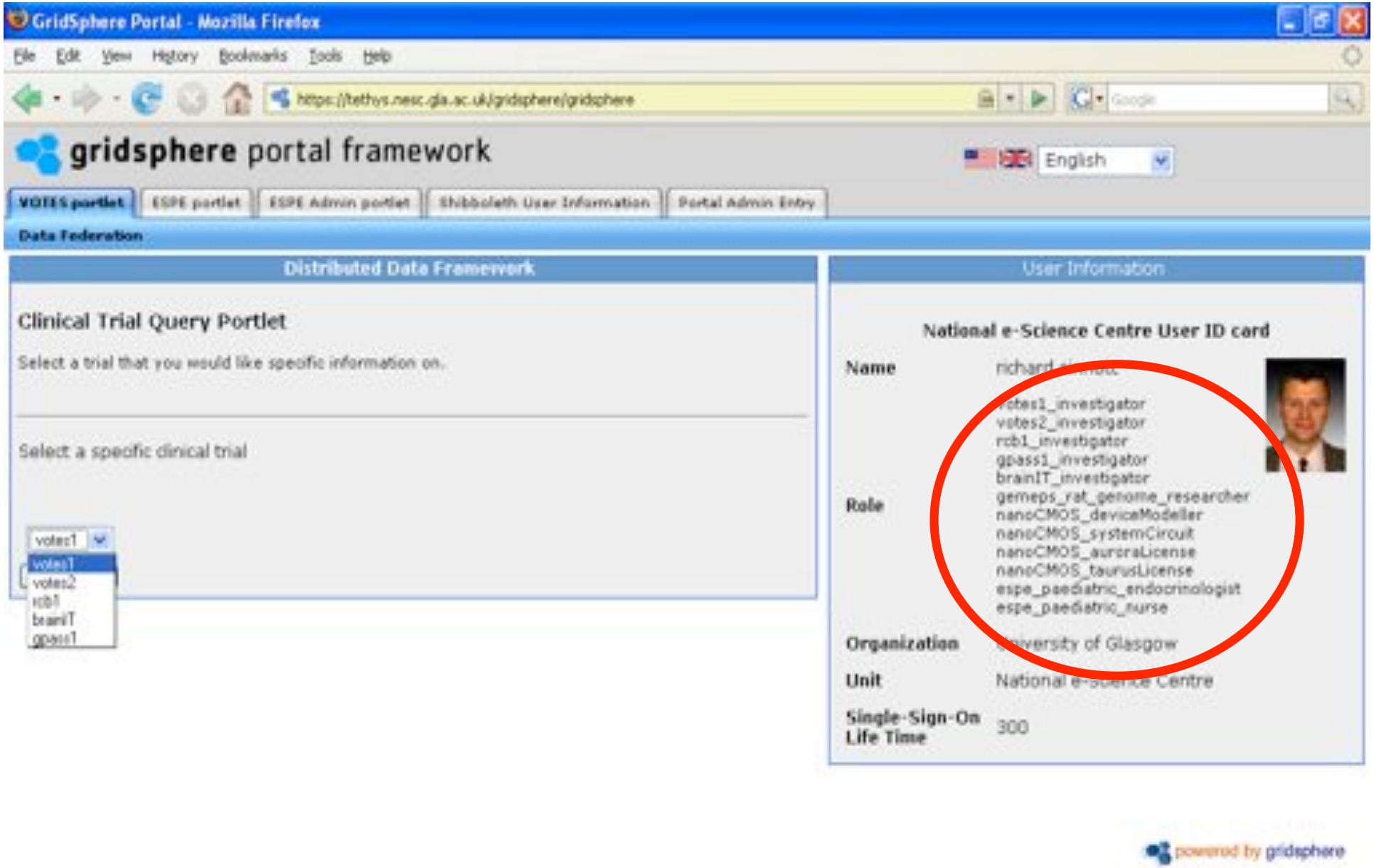
- **I can do authorisation but I want single-sign on to lots of distributed resources**
  - **Browser allows to keep session information so can access other resources without signing in again**
    - Provided authorisation information valid for different service providers
      - Each service provider completely autonomous
    - Can configure attribute release/attribute acceptance policies per identity provider/service provider

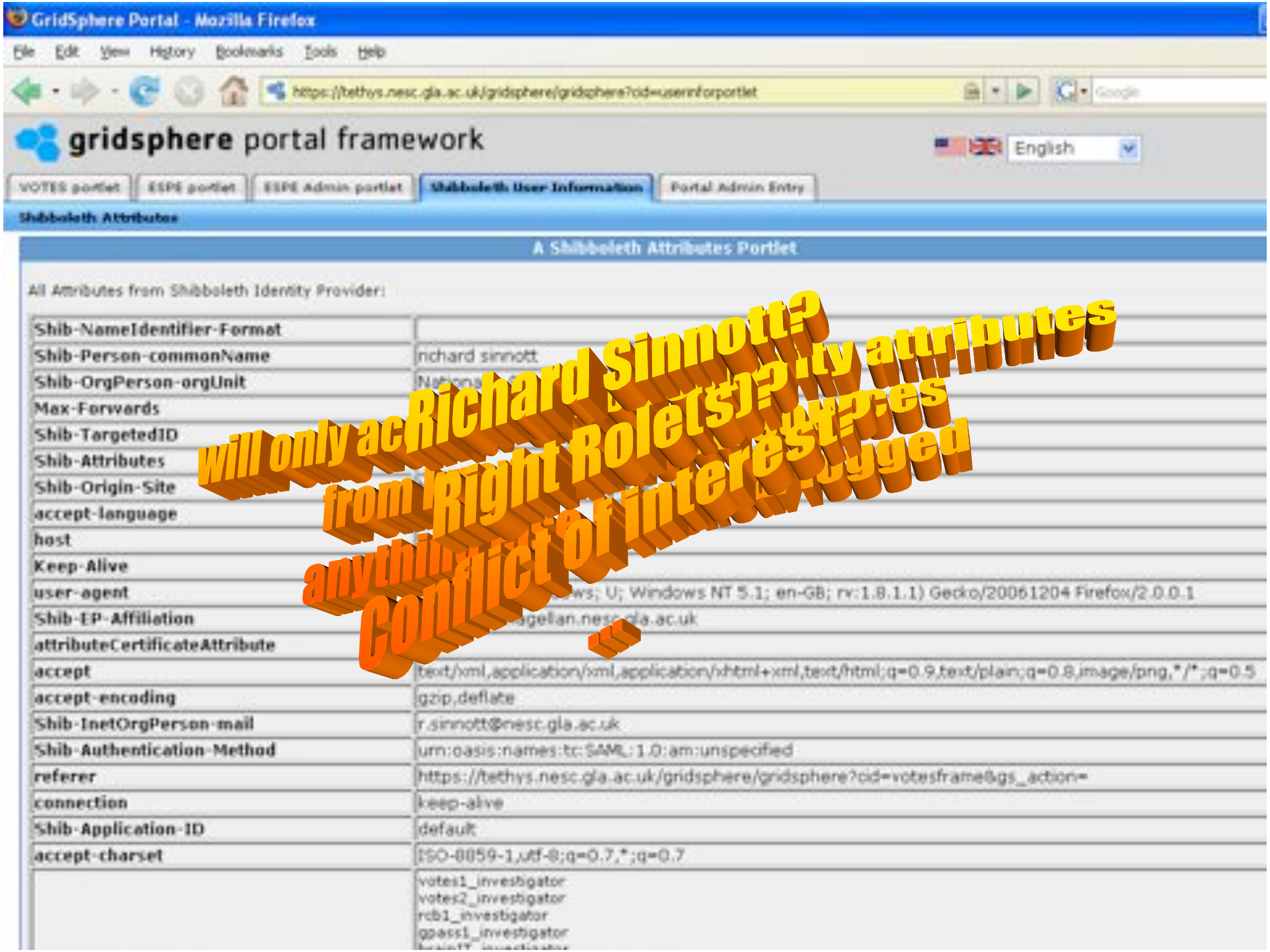
# Single Sign-On Demonstration:

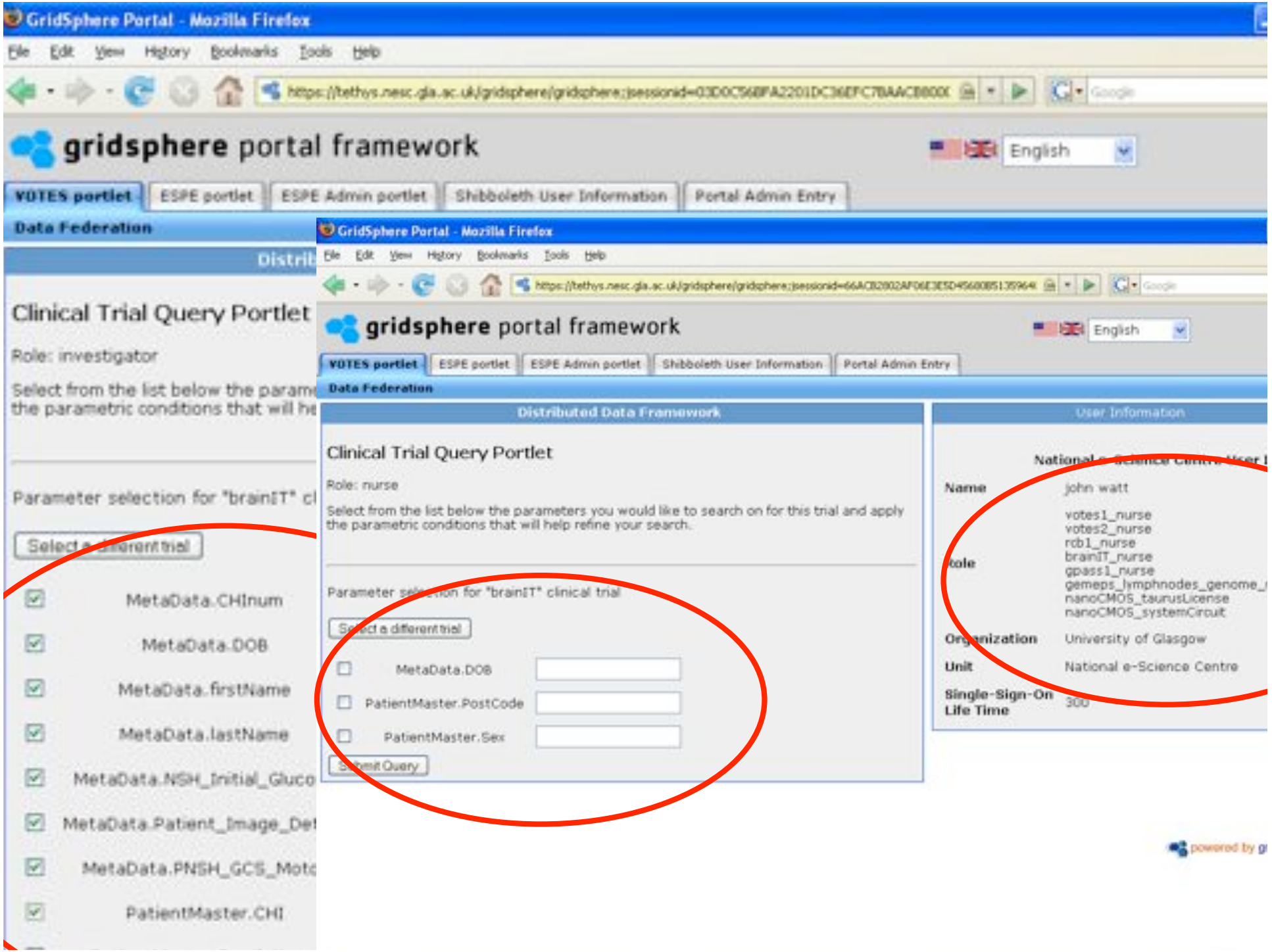
# Step 1: User attempts to access clinical trials portal

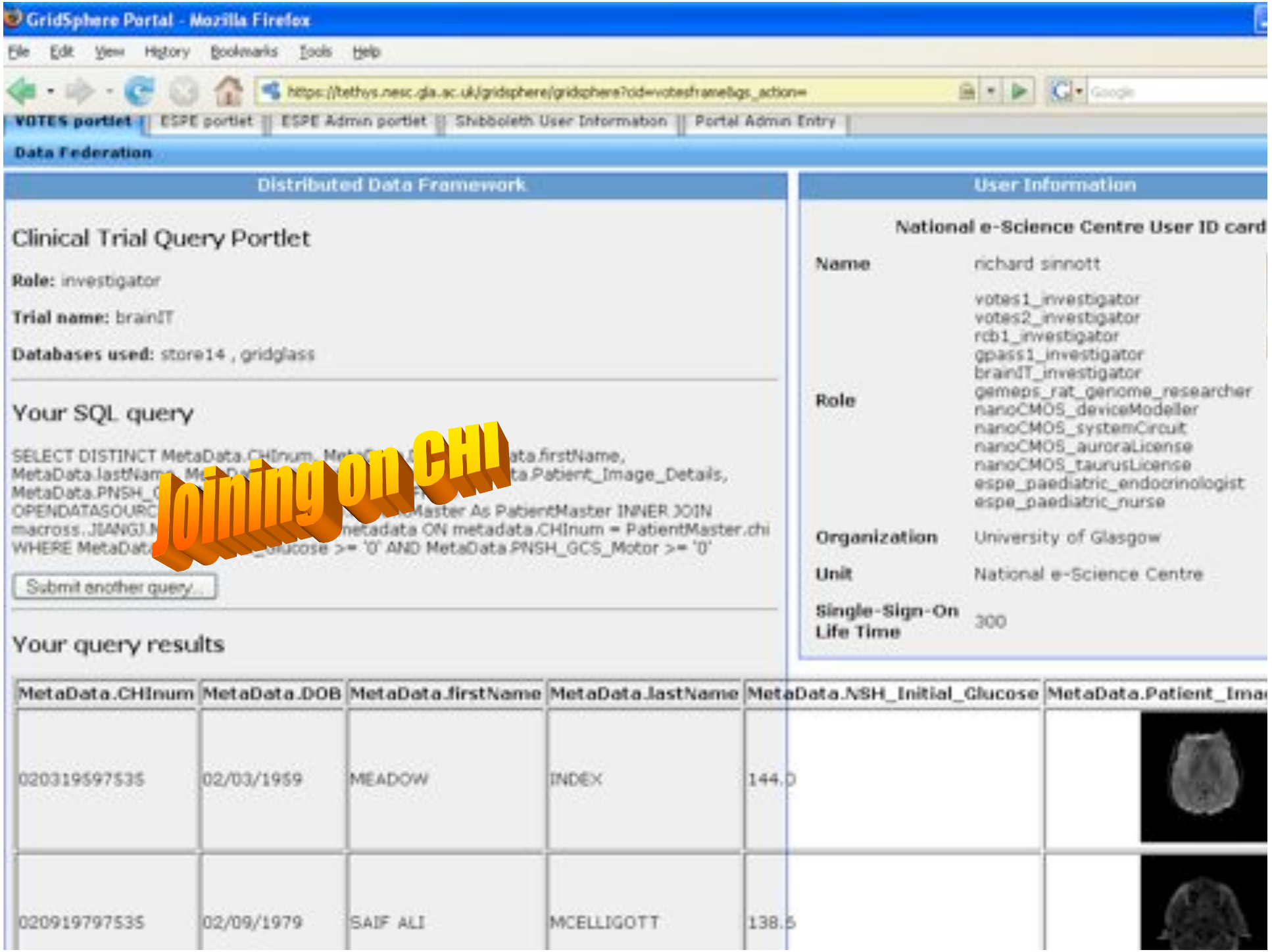

Select your home organisation - Mozilla Firefox
File Edit View History Bookmarks Tools Help
The UK Access Management Federation
Select your home organisation
Selection options
The service you are trying to reach requires that you authenticate with your home organization. Please select an organization using one of the methods below.
Choose from list
AHDS: King's College
Select
Search
Matu
Metaleth
MIMAS
NeSC Glasgow
Newcastle
Newcastle - Medical Sciences
Nottingham Trent University
OeRC Test
Oxford University Computing Services (Test)
ProtectNetwork
RAGS
RSC South West
SAFAPI UKDA (origin)
Salford Software
SDSS
SDSS Causewayside
SDSS Causewayside (1.2)
SDSS slioch-test
SDSS Thirlestane (CA test)
SDSS TypeKey Bridge

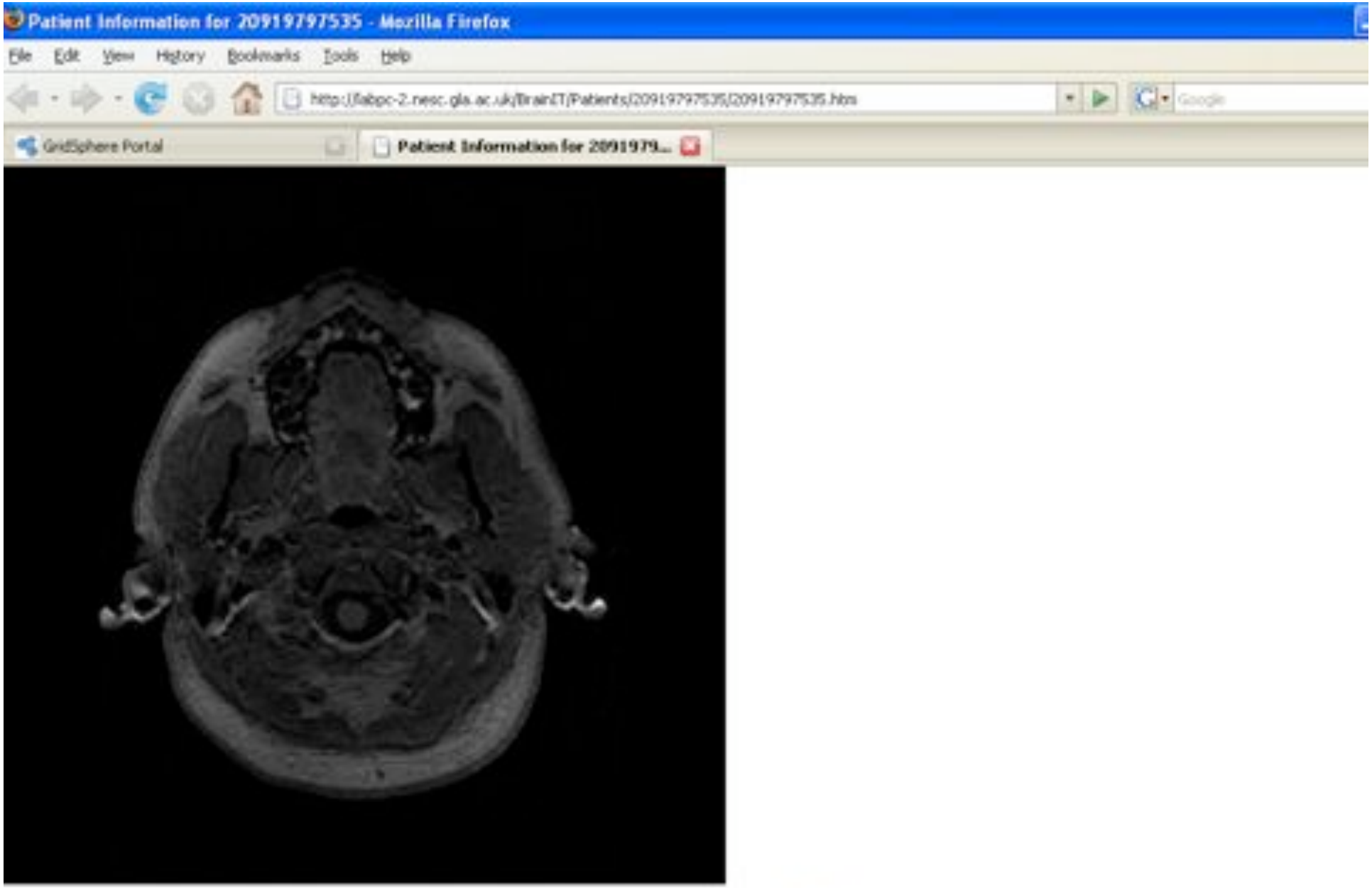

Select your home organisation - Mozilla Firefox
File Edit View History Bookmarks Tools Help
The UK Access Management Federation
Select your home organisation
Selection options
The service you are trying to reach requires that you authenticate with your home organization. Please select
Choose from list
NeSC Glasgow
Remember for session
Search by keyword
Authentication Required
Enter username and password for "NeSC Glasgow Identity Provider" at https://magellan.nesc.gla.ac.uk.
User Name:
roslm
Password:
Use Password Manager to remember this password.
OK
Cancel
Need assistance? Visit the UK Federation web site.


GridSphere Portal - Mozilla Firefox
File Edit View History Bookmarks Tools Help
https://tethys.nesc.gla.ac.uk/gridsphere/gridsphere
gridsphere portal framework
English
VOTES portlet
ESPE portlet
ESPE Admin portlet
Shibboleth User Information
Portal Admin Entry
Data Federation
Distributed Data Framework
Clinical Trial Query Portlet
Select a trial that you would like specific information on.
Select a specific clinical trial
votes1
votes1
votes2
rcb1
brainIT
gpass1
User Information
National e-Science Centre User ID card
Name
votes1_investigator
votes2_investigator
rcb1_investigator
gpass1_investigator
brainIT_investigator
gemeps_rat_genome_researcher
nanoCMOS_deviceModeller
nanoCMOS_systemCircuit
nanoCMOS_auroraLicense
nanoCMOS_taurusLicense
espe_paediatric_endocrinologist
espe_paediatric_nurse
Role
Organization
University of Glasgow
Unit
National e-Science Centre
Single-Sign-On Life Time
300
powered by gridsphere


GridSphere Portal - Mozilla Firefox
File Edit View History Bookmarks Tools Help
https://tethys.nesc.gla.ac.uk/gridsphere/gridsphere?cid=userinfoportlet
gridsphere portal framework
English
VOTES portlet
ESPE portlet
ESPE Admin portlet
Shibboleth User Information
Portal Admin Entry
Shibboleth Attributes
A Shibboleth Attributes Portlet
All Attributes from Shibboleth Identity Provider:
Shib-NameIdentifier-Format
Shib-Person-commonName
richard sinnott
Shib-OrgPerson-orgUnit
Max-Forwards
Shib-TargetedID
Shib-Attributes
Shib-Origin-Site
accept-language
host
Keep-Alive
user-agent
Windows; U; Windows NT 5.1; en-GB; rv:1.8.1.1) Gecko/20061204 Firefox/2.0.0.1
Shib-EP-Affiliation
magellan.nesc.gla.ac.uk
attributeCertificateAttribute
accept
text/xml,application/xml,application/xhtml+xml,text/html;q=0.9,text/plain;q=0.8,image/png,*/*;q=0.5
accept-encoding
gzip,deflate
Shib-InetOrgPerson-mail
r.sinnott@nesc.gla.ac.uk
Shib-Authentication-Method
urn:oasis:names:tc:SAML:1.0:am:unspecified
referer
https://tethys.nesc.gla.ac.uk/gridsphere/gridsphere?cid=votesframe&gs_action=
connection
keep-alive
Shib-Application-ID
default
accept-charset
ISO-8859-1,utf-8;q=0.7,*;q=0.7
votes1_investigator
votes2_investigator
rcb1_investigator
gpass1_investigator
will only ac
from
anythi
Richard Sinnott?
Right Role[s]?
Conflict of interest?
ity attributes
es
ogged

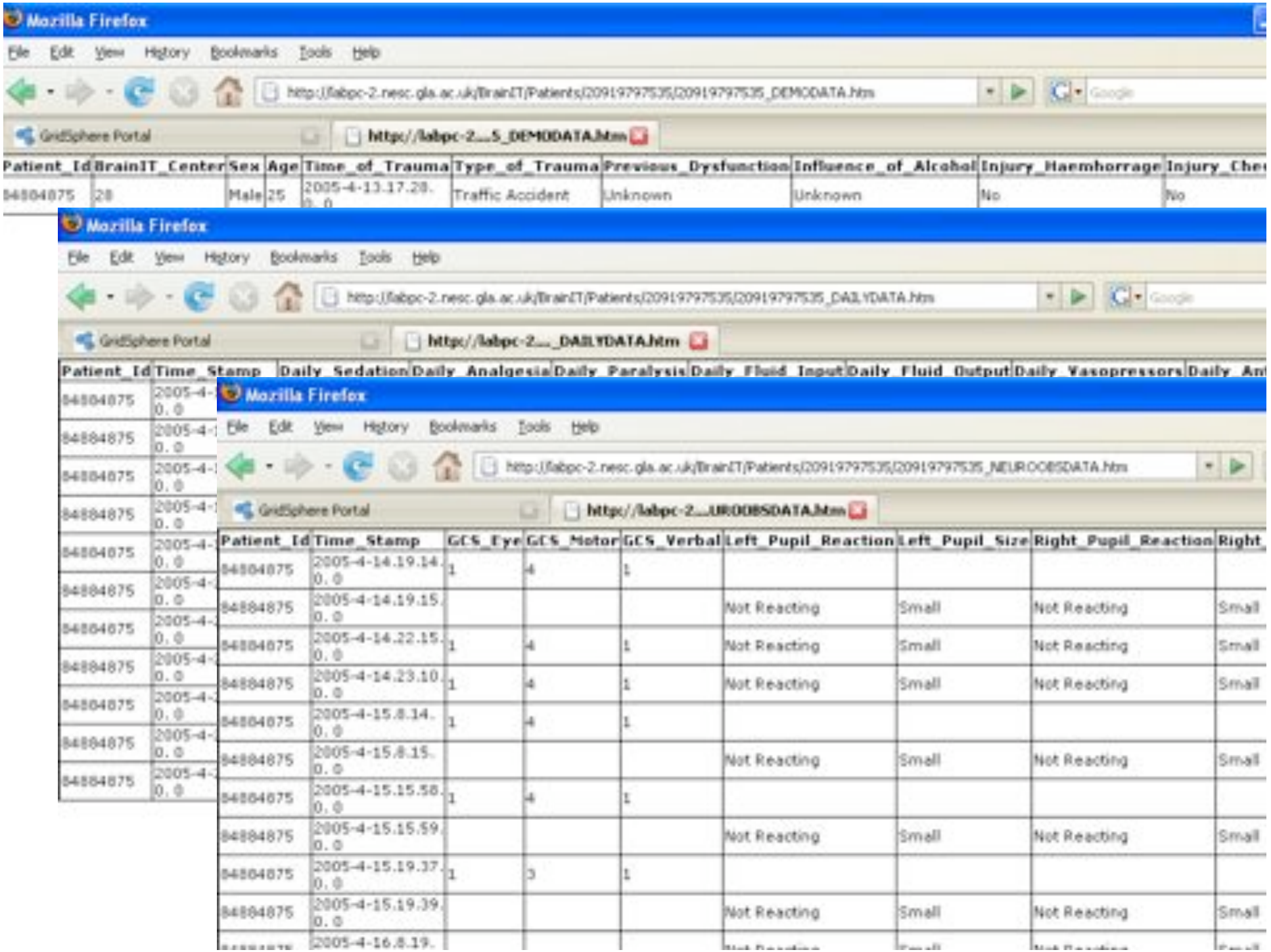

GridSphere Portal - Mozilla Firefox
File Edit View History Bookmarks Tools Help
gridsphere portal framework
English
VOTES portlet
ESPE portlet
ESPE Admin portlet
Shibboleth User Information
Portal Admin Entry
Data Federation
Clinical Trial Query Portlet
Role: investigator
Select from the list below the parame
the parametric conditions that will he
Parameter selection for "brainIT" cl
Select a different trial
MetaData.CHInum
MetaData.DOB
MetaData.firstName
MetaData.lastName
MetaData.NSH_Initial_Gluco
MetaData.Patient_Image_Det
MetaData.PNSH_GCS_Moto
PatientMaster.CHI
GridSphere Portal - Mozilla Firefox
File Edit View History Bookmarks Tools Help
gridsphere portal framework
English
VOTES portlet
ESPE portlet
ESPE Admin portlet
Shibboleth User Information
Portal Admin Entry
Data Federation
Distributed Data Framework
Clinical Trial Query Portlet
Role: nurse
Select from the list below the parameters you would like to search on for this trial and apply the parametric conditions that will help refine your search.
Parameter selection for "brainIT" clinical trial
Select a different trial
MetaData.DOB
PatientMaster.PostCode
PatientMaster.Sex
Submit Query
User Information
Name
john watt
Role
votes1_nurse
votes2_nurse
rcb1_nurse
brainIT_nurse
gpass1_nurse
gemeps_lymphnodes_genome_
nanoCMOS_taurusLicense
nanoCMOS_systemCircuit
Organization
University of Glasgow
Unit
National e-Science Centre
Single-Sign-On Life Time
300


GridSphere Portal - Mozilla Firefox
File Edit View History Bookmarks Tools Help
https://tethys.nesc.gla.ac.uk/gridsphere/gridsphere?cid=votesframe&gs_action=
VOTES portlet
ESPE portlet
ESPE Admin portlet
Shibboleth User Information
Portal Admin Entry
Data Federation
Distributed Data Framework
Clinical Trial Query Portlet
Role: investigator
Trial name: brainIT
Databases used: store14 , gridglass
Your SQL query
Joining on CHI
Submit another query...
Your query results
MetaData.CHInum
MetaData.DOB
MetaData.firstName
MetaData.lastName
MetaData.PNSH_Initial_Glucose
MetaData.Patient_Ima
020319597535
02/03/1959
MEADOW
INDEX
020919797535
02/09/1979
SAIF ALI
MCELLIGOTT
User Information
National e-Science Centre User ID card
Name
richard sinnott
Role
votes1_investigator
votes2_investigator
rcb1_investigator
gpass1_investigator
brainIT_investigator
gemeps_rat_genome_researcher
nanoCMOS_deviceModeller
nanoCMOS_systemCircuit
nanoCMOS_auroraLicense
nanoCMOS_taurusLicense
espe_paediatric_endocrinologist
espe_paediatric_nurse
Organization
University of Glasgow
Unit
National e-Science Centre
Single-Sign-On Life Time
300




To analyze the patient brain images on DICOM software, download the patient files from here (Please right click the mouse and select 'Save Link As...').
One of the free version of DICOM software, called *DicomWorks*, can be download from here.
The complete information about patient *04804075* is displayed below:

- **Daily Data** (values taken once per day)
- **Demo Data** (study Admit Document used in all projects)



Mozilla Firefox

File Edit View History Bookmarks Tools Help

http://labpc-2.nesc.gla.ac.uk/BrainIT/Patients/20919797535/20919797535_DEMODATA.htm

GridSphere Portal

http/labpc-2...S_DEMODATA.htm

| Patient_Id | BrainIT_Center | Sex | Age | Time_of_Trauma | Type_of_Trauma | Previous_Dysfunction | Influence_of_Alcohol | Injury_Haemhorrage | Injury_Che |
|---|---|---|---|---|---|---|---|---|---|
| 84884875 | 28 | Male | 25 | 2005-4-13.17.28. 0. 0 | Traffic Accident | Unknown | Unknown | No | No |

Mozilla Firefox

File Edit View History Bookmarks Tools Help

http://labpc-2.nesc.gla.ac.uk/BrainIT/Patients/20919797535/20919797535_DAILYDATA.htm

GridSphere Portal

http/labpc-2..._DAILYDATA.htm

| Patient_Id | Time_Stamp | Daily_Sedation | Daily_Analgesia | Daily_Paralysis | Daily_Fluid_Input | Daily_Fluid_Output | Daily_Vasopressors | Daily_An |
|---|---|---|---|---|---|---|---|---|
| 84884875 | 2005-4-... 0. 0 | | | | | | | |
| 84884875 | 2005-4-... 0. 0 | | | | | | | |
| 84884875 | 2005-4-... 0. 0 | | | | | | | |
| 84884875 | 2005-4-... 0. 0 | | | | | | | |
| 84884875 | 2005-4-... 0. 0 | | | | | | | |
| 84884875 | 2005-4-... 0. 0 | | | | | | | |
| 84884875 | 2005-4-... 0. 0 | | | | | | | |
| 84884875 | 2005-4-... 0. 0 | | | | | | | |
| 84884875 | 2005-4-... 0. 0 | | | | | | | |
| 84884875 | 2005-4-... 0. 0 | | | | | | | |

Mozilla Firefox

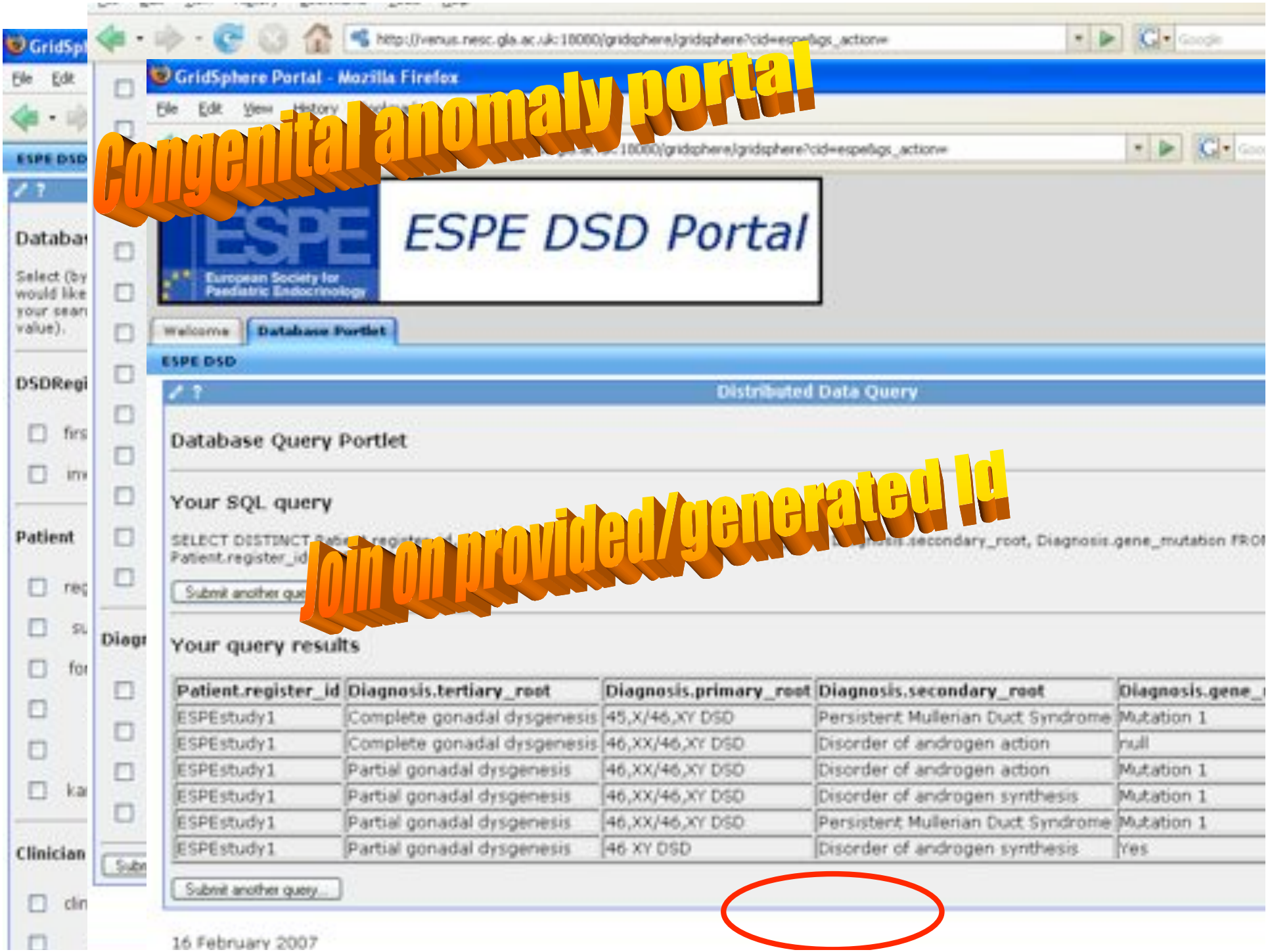
File Edit View History Bookmarks Tools Help

http://labpc-2.nesc.gla.ac.uk/BrainIT/Patients/20919797535/20919797535_NEUROOBSDATA.htm

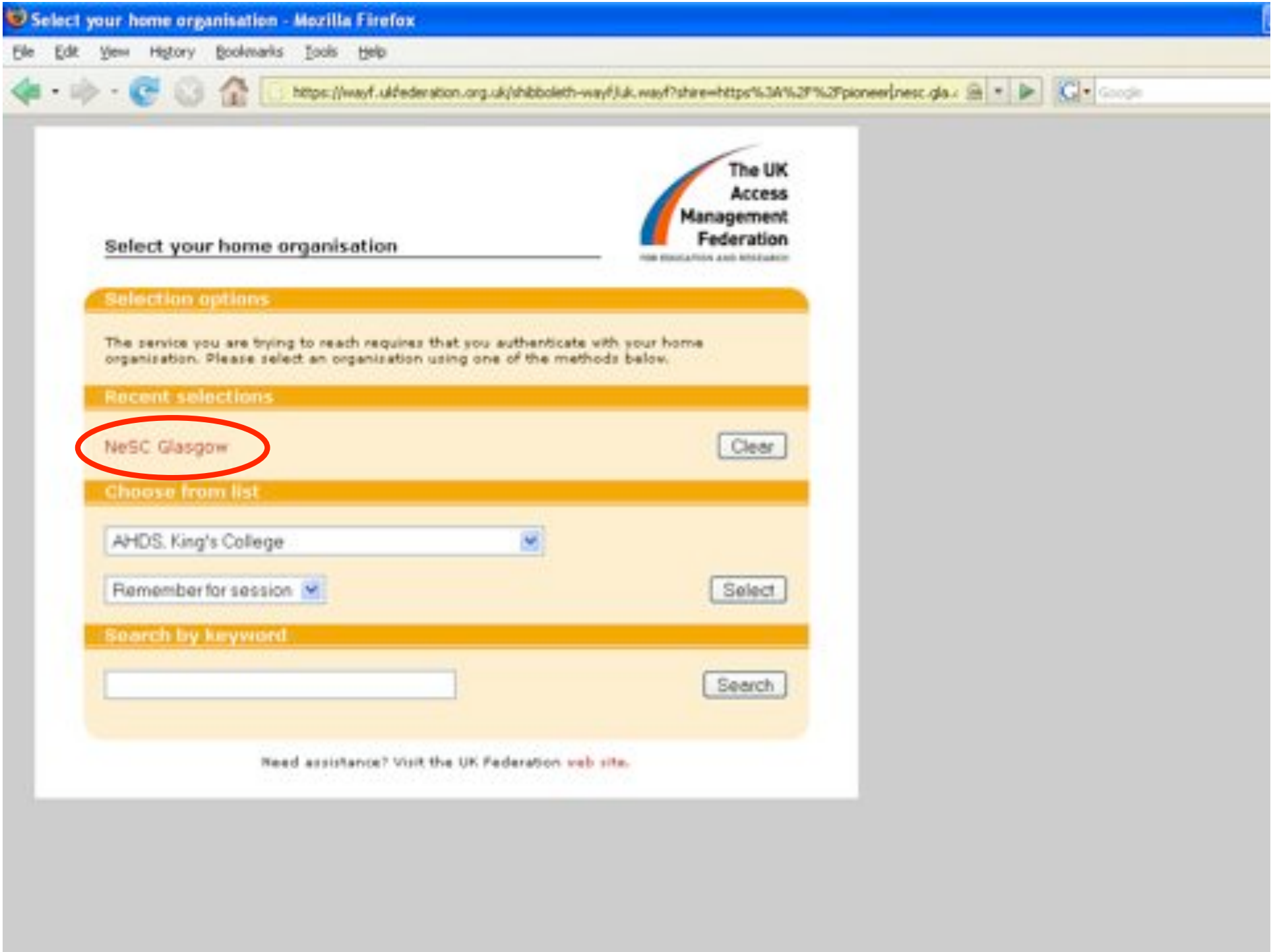
GridSphere Portal

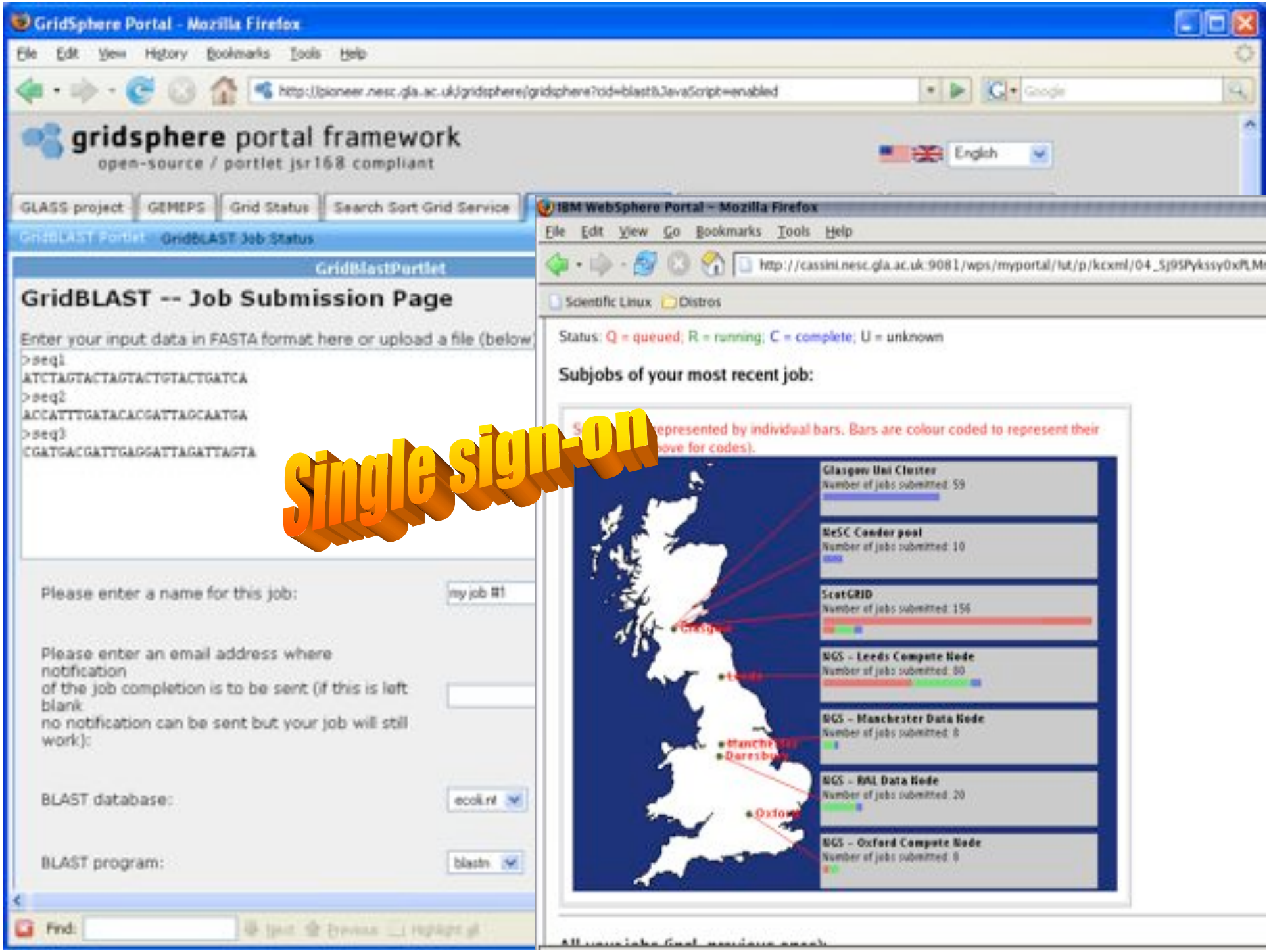
http/labpc-2...UROOBSDATA.htm

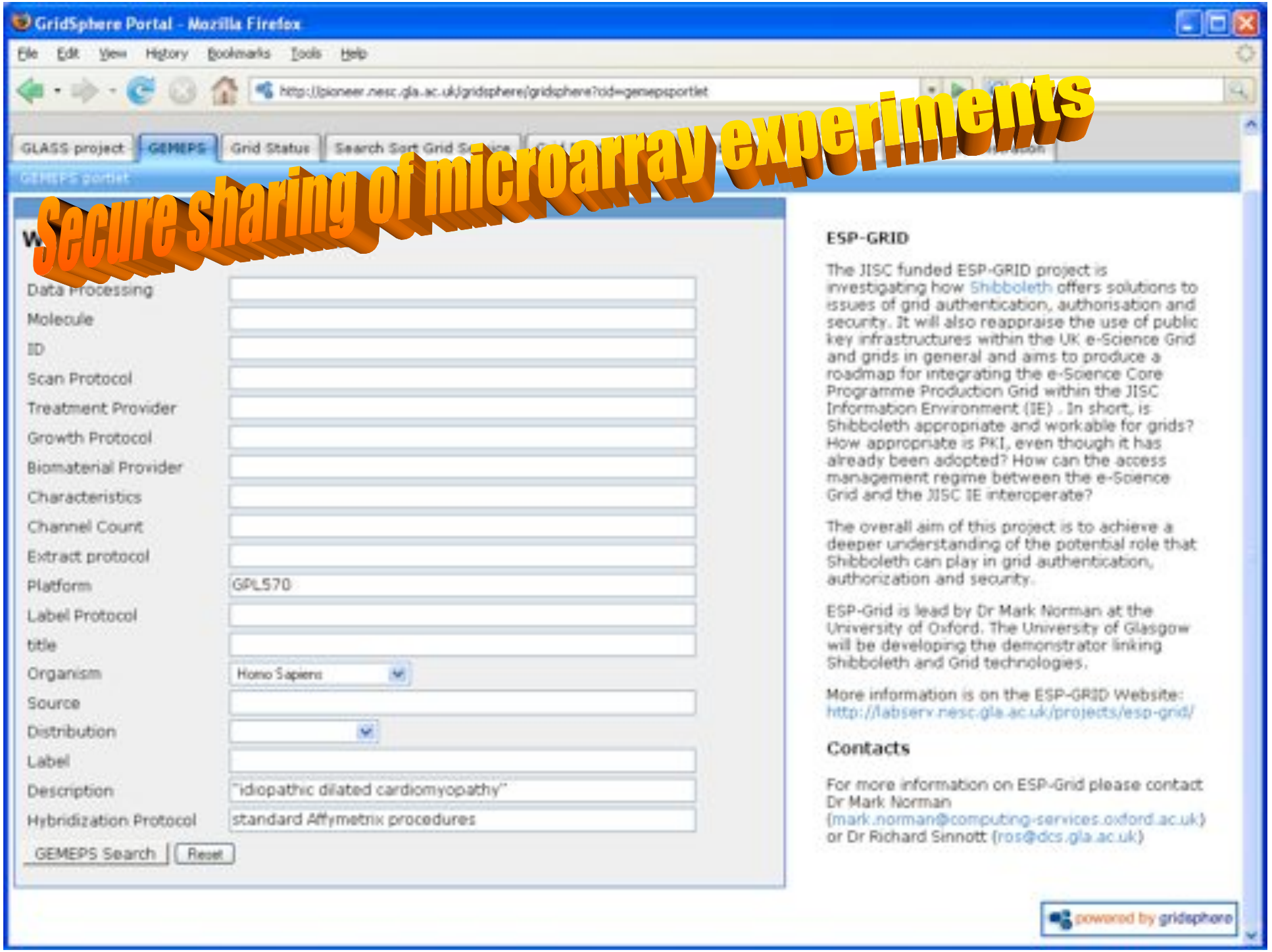
| Patient_Id | Time_Stamp | GCS_Eye | GCS_Motor | GCS_Verbal | Left_Pupil_Reaction | Left_Pupil_Size | Right_Pupil_Reaction | Right_ |
|---|---|---|---|---|---|---|---|---|
| 84884875 | 2005-4-14.19.14. 0. 0 | 1 | 4 | 1 | | | | |
| 84884875 | 2005-4-14.19.15. 0. 0 | | | | Not Reacting | Small | Not Reacting | Small |
| 84884875 | 2005-4-14.22.15. 0. 0 | 1 | 4 | 1 | Not Reacting | Small | Not Reacting | Small |
| 84884875 | 2005-4-14.23.10. 0. 0 | 1 | 4 | 1 | Not Reacting | Small | Not Reacting | Small |
| 84884875 | 2005-4-15.8.14. 0. 0 | 1 | 4 | 1 | | | | |
| 84884875 | 2005-4-15.8.15. 0. 0 | | | | Not Reacting | Small | Not Reacting | Small |
| 84884875 | 2005-4-15.15.58. 0. 0 | 1 | 4 | 1 | | | | |
| 84884875 | 2005-4-15.15.59. 0. 0 | | | | Not Reacting | Small | Not Reacting | Small |
| 84884875 | 2005-4-15.19.37. 0. 0 | 1 | 5 | 1 | | | | |
| 84884875 | 2005-4-15.19.39. 0. 0 | | | | Not Reacting | Small | Not Reacting | Small |
| 84884875 | 2005-4-16.8.19. | | | | | | | |

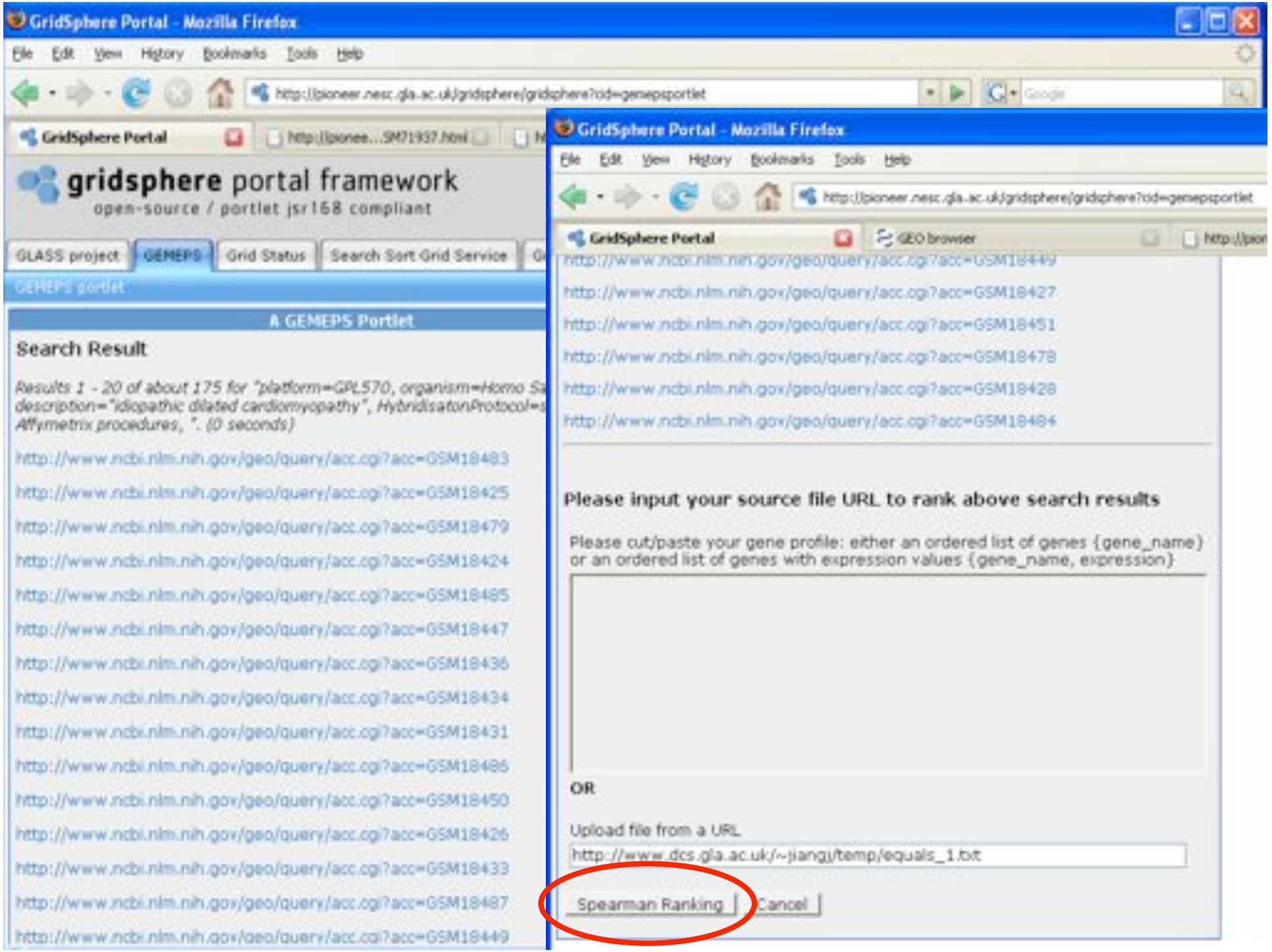


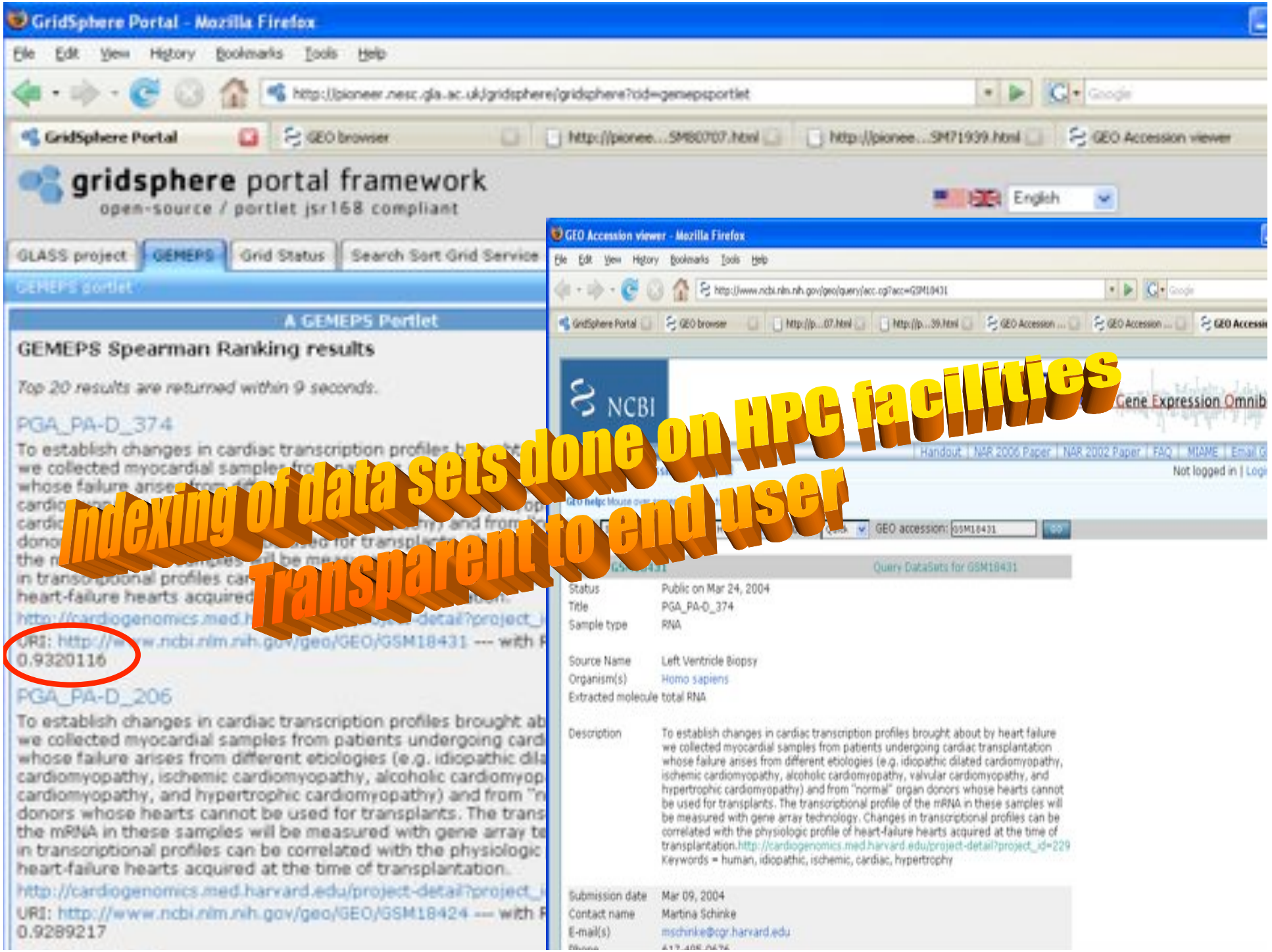

| Patient.register_id | Diagnosis.tertiary_root | Diagnosis.primary_root | Diagnosis.secondary_root | Diagnosis.gene_ |
|---|---|---|---|---|
| ESPEstudy1 | Complete gonadal dysgenesis | 45,X/46,XY DSD | Persistent Mullerian Duct Syndrome | Mutation 1 |
| ESPEstudy1 | Complete gonadal dysgenesis | 46,XX/46,XY DSD | Disorder of androgen action | null |
| ESPEstudy1 | Partial gonadal dysgenesis | 46,XX/46,XY DSD | Disorder of androgen action | Mutation 1 |
| ESPEstudy1 | Partial gonadal dysgenesis | 46,XX/46,XY DSD | Disorder of androgen synthesis | Mutation 1 |
| ESPEstudy1 | Partial gonadal dysgenesis | 46,XX/46,XY DSD | Persistent Mullerian Duct Syndrome | Mutation 1 |
| ESPEstudy1 | Partial gonadal dysgenesis | 46 XY DSD | Disorder of androgen synthesis | Yes |


Select your home organisation - Mozilla Firefox
File Edit View History Bookmarks Tools Help
The UK Access Management Federation
Select your home organisation
Selection options
The service you are trying to reach requires that you authenticate with your home organization. Please select an organization using one of the methods below.
Recent selections
NeSC Glasgow
Clear
Choose from list
AHDS, King's College
Remember for session
Select
Search by keyword
Search
Need assistance? Visit the UK Federation web site.


GridSphere Portal - Mozilla Firefox
gridsphere portal framework
open-source / portlet jsr168 compliant
English
GLASS project
GEMEPS
Grid Status
Search Sort Grid Service
GridBLAST Portlet
GridBLAST Job Status
GridBlastPortlet
GridBLAST -- Job Submission Page
Enter your input data in FASTA format here or upload a file (below)
>seq1
ATCTAGTACTAGTACTGTACTGATCA
>seq2
ACCATTTGATACACGATTAGCAATGA
>seq3
CGATGACGATTGAGGATTAGATTAGTA
Please enter a name for this job:
my job #1
Please enter an email address where notification
of the job completion is to be sent (if this is left blank
no notification can be sent but your job will still work):
BLAST database:
ecoli.nt
BLAST program:
blastn
Find:
IBM WebSphere Portal - Mozilla Firefox
Scientific Linux
Distros
Status: Q = queued; R = running; C = complete; U = unknown
Subjobs of your most recent job:
Glasgow Uni Cluster
Number of jobs submitted: 59
NeSC Condor pool
Number of jobs submitted: 10
ScotGRID
Number of jobs submitted: 156
NGS - Leeds Compute Node
Number of jobs submitted: 80
NGS - Manchester Data Node
Number of jobs submitted: 8
NGS - RAL Data Node
Number of jobs submitted: 20
NGS - Oxford Compute Node
Number of jobs submitted: 8
Single sign-on


GridSphere Portal - Mozilla Firefox
File Edit View History Bookmarks Tools Help
GLASS project
GEMEPS
Grid Status
Search Sort Grid
GEMEPS portlet
Secure sharing of microarray experiments
Data Processing
Molecule
ID
Scan Protocol
Treatment Provider
Growth Protocol
Biomaterial Provider
Characteristics
Channel Count
Extract protocol
Platform
GPL570
Label Protocol
title
Organism
Homo Sapiens
Source
Distribution
Label
Description
"idiopathic dilated cardiomyopathy"
Hybridization Protocol
standard Affymetrix procedures
GEMEPS Search
Reset
ESP-GRID
The JISC funded ESP-GRID project is investigating how Shibboleth offers solutions to issues of grid authentication, authorisation and security. It will also reappraise the use of public key infrastructures within the UK e-Science Grid and grids in general and aims to produce a roadmap for integrating the e-Science Core Programme Production Grid within the JISC Information Environment (IE) . In short, is Shibboleth appropriate and workable for grids? How appropriate is PKI, even though it has already been adopted? How can the access management regime between the e-Science Grid and the JISC IE interoperate?
The overall aim of this project is to achieve a deeper understanding of the potential role that Shibboleth can play in grid authentication, authorization and security.
ESP-Grid is lead by Dr Mark Norman at the University of Oxford. The University of Glasgow will be developing the demonstrator linking Shibboleth and Grid technologies.
More information is on the ESP-GRID Website: http://labserv.nesc.gla.ac.uk/projects/esp-grid/
Contacts
For more information on ESP-Grid please contact Dr Mark Norman (mark.norman@computing-services.oxford.ac.uk) or Dr Richard Sinnott (ros@dcs.gla.ac.uk)
powered by gridsphere


GridSphere Portal - Mozilla Firefox
File Edit View History Bookmarks Tools Help
http://pioneer.nesc.gla.ac.uk/gridsphere/gridsphere?cid=genepsportlet
GridSphere Portal
gridsphere portal framework
open-source / portlet jsr168 compliant
GLASS project
GEMEPS
Grid Status
Search Sort Grid Service
A GEMEPS Portlet
Search Result
Results 1 - 20 of about 175 for "platform=GPL570, organism=Homo Sa
description="idiopathic dilated cardiomyopathy", HybridisatonProtocol=
Affymetrix procedures, ". (0 seconds)
http://www.ncbi.nlm.nih.gov/geo/query/acc.cgi?acc=GSM18483
http://www.ncbi.nlm.nih.gov/geo/query/acc.cgi?acc=GSM18425
http://www.ncbi.nlm.nih.gov/geo/query/acc.cgi?acc=GSM18479
http://www.ncbi.nlm.nih.gov/geo/query/acc.cgi?acc=GSM18424
http://www.ncbi.nlm.nih.gov/geo/query/acc.cgi?acc=GSM18485
http://www.ncbi.nlm.nih.gov/geo/query/acc.cgi?acc=GSM18447
http://www.ncbi.nlm.nih.gov/geo/query/acc.cgi?acc=GSM18436
http://www.ncbi.nlm.nih.gov/geo/query/acc.cgi?acc=GSM18434
http://www.ncbi.nlm.nih.gov/geo/query/acc.cgi?acc=GSM18431
http://www.ncbi.nlm.nih.gov/geo/query/acc.cgi?acc=GSM18486
http://www.ncbi.nlm.nih.gov/geo/query/acc.cgi?acc=GSM18450
http://www.ncbi.nlm.nih.gov/geo/query/acc.cgi?acc=GSM18426
http://www.ncbi.nlm.nih.gov/geo/query/acc.cgi?acc=GSM18433
http://www.ncbi.nlm.nih.gov/geo/query/acc.cgi?acc=GSM18487
http://www.ncbi.nlm.nih.gov/geo/query/acc.cgi?acc=GSM18449
GridSphere Portal - Mozilla Firefox
File Edit View History Bookmarks Tools Help
http://pioneer.nesc.gla.ac.uk/gridsphere/gridsphere?cid=genepsportlet
GridSphere Portal
GEO browser
http://www.ncbi.nlm.nih.gov/geo/query/acc.cgi?acc=GSM18427
http://www.ncbi.nlm.nih.gov/geo/query/acc.cgi?acc=GSM18451
http://www.ncbi.nlm.nih.gov/geo/query/acc.cgi?acc=GSM18478
http://www.ncbi.nlm.nih.gov/geo/query/acc.cgi?acc=GSM18428
http://www.ncbi.nlm.nih.gov/geo/query/acc.cgi?acc=GSM18484
Please input your source file URL to rank above search results
Please cut/paste your gene profile: either an ordered list of genes {gene_name}
or an ordered list of genes with expression values {gene_name, expression}
OR
Upload file from a URL
http://www.dcs.gla.ac.uk/~jiangj/temp/equals_1.txt
Spearman Ranking
Cancel


GridSphere Portal - Mozilla Firefox
gridsphere portal framework
open-source / portlet jsr168 compliant
GLASS project
GEMEPS
Grid Status
Search Sort Grid Service
A GEMEPS Portlet
GEMEPS Spearman Ranking results
Top 20 results are returned within 9 seconds.
PGA_PA-D_374
0.9320116
PGA_PA-D_206
0.9289217
GEO Accession viewer - Mozilla Firefox
NCBI
Gene Expression Omnibus
GEO accession: GSM18431
Query DataSets for GSM18431
Status Public on Mar 24, 2004
Title PGA_PA-D_374
Sample type RNA
Source Name Left Ventricle Biopsy
Organism(s) Homo sapiens
Extracted molecule total RNA
Submission date Mar 09, 2004
Contact name Martina Schinke
E-mail(s) mschinke@cgr.harvard.edu
Indexing of data sets done on HPC facilities
Transparent to end user

# Conclusions

- **Numerous application domains exploring e-Science/Grid technologies**
- **Consolidation of know-how/technologies essential**
  - **EGEE**
  - **OMII**
  - **UK e-Science task forces (ETF, STF, ATF, …)**
  - **NDCC**
  - **NeSC**
- **Do we know how best to build Grids?**
  - **Different domains coming up with own ways of building Grids**
    - OGSA needed asap
  - **Clear that various domains have issues which must be resolved before Grid can make significant** and long lasting **impact**
- **NeSC Glasgow is leader in security/life sciences but still lots to do/learn…**

# Conclusions …ctd

- Many other projects feeding Scottish efforts
  - **Scottish Grid Service**
  - **Scottish Bioinformatics Research Network**
    - Biochemical pathway tools, drug discovery portals, …
  - **Shibboleth access to Geographical Information Systems**
  - **Generation Scotland Scottish Family Health Study**
  - **Grid Enabled Occupational Data Environment**
    - Social aspects/classification important
  - **Many other projects developing/improving tools for Grid security**
    - Building on Shibboleth efforts!
  - **Scottish University Life Science Association (SULSA)**

# Questions …?