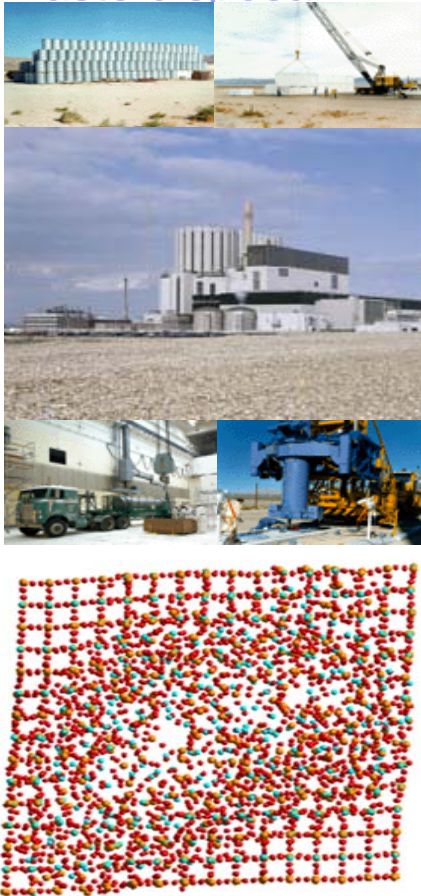


An Integrated Computing and Data Environment for Environmental Science

Kerstin Kleese van Dam

Lisa Blanshard, Rik Tyer

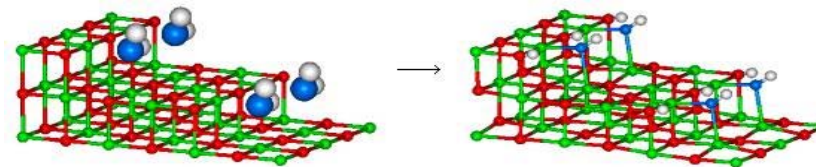
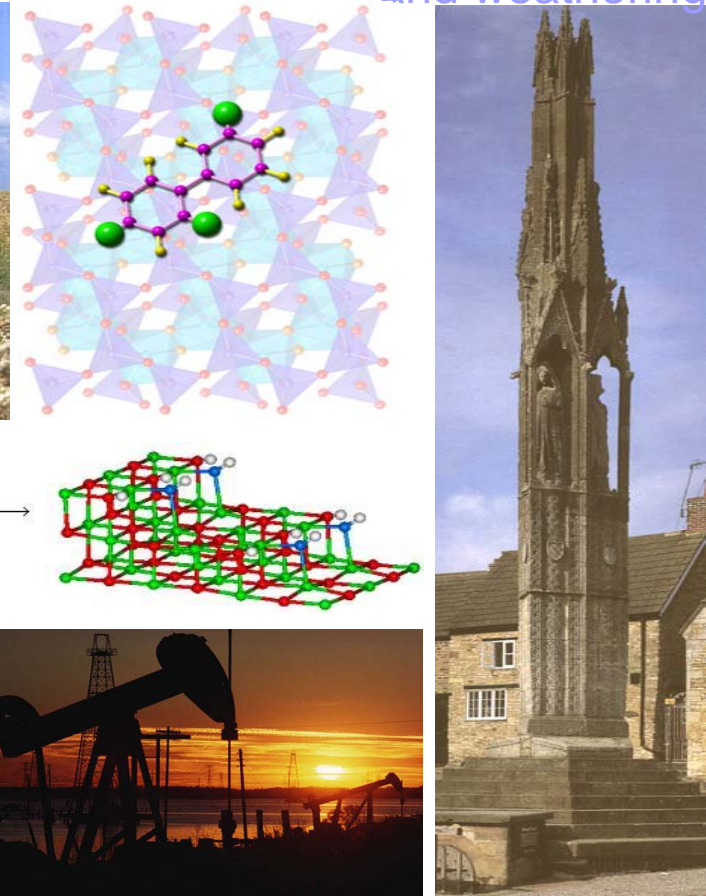
Radioactive
waste disposal



Pollution: molecules and
atoms on mineral surfaces



Crystal dissolution
and weathering



Crystal growth and
scale inhibition





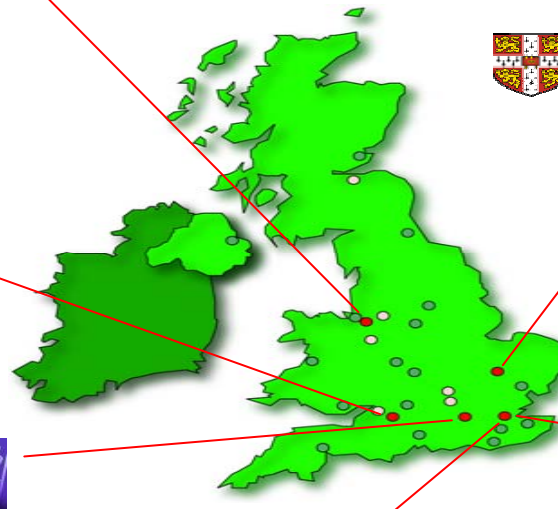
CCLRC Daresbury



**UNIVERSITY OF
CAMBRIDGE**



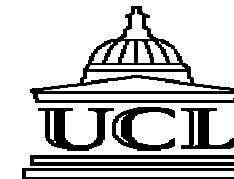
**UNIVERSITY OF
BATH**

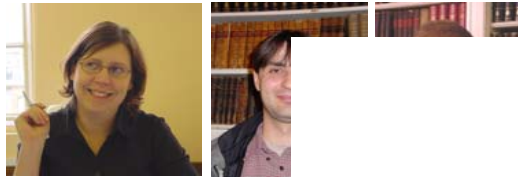
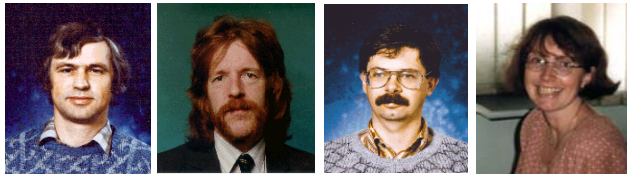


**University of
Reading**



Royal Institution

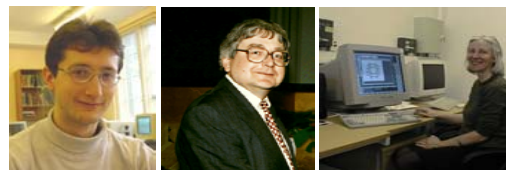
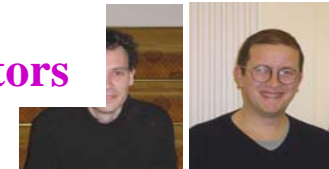




11 Principle Investigators

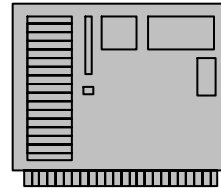
12 PDRAs

Many other direct and indirect Collaborators

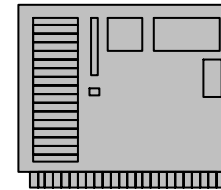


HPCx

4 Node IBM Database System



CCLRC Daresbury



16 Node Linux Cluster

40 Node Linux Cluster

25 Node Condor Cluster

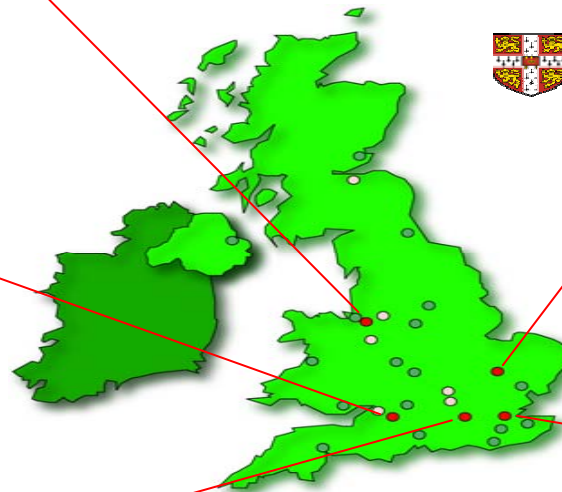
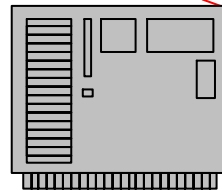


UNIVERSITY OF CAMBRIDGE



UNIVERSITY OF BATH

16 Node Linux Cluster



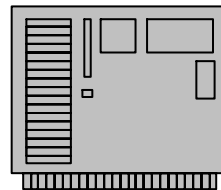
16 Node Linux Cluster

910 Node Condor Pool



University of Reading

24 Node IBM Cluster



+ National Grid Service at Manchester, Leeds, Oxford and CCLRC

10 Different sites and administrations – user names, passwords, batch systems

13 Different Computers with varying operating systems, compilers, file systems, licenses

Question:

How to enable scientists to use these resources to their full extend, without spending their days locked in administration?

Single Sign On – to all resources – computing, data and application - > x509 certificates for authentication + separate authorisation certificates

One Job Submission Interface – to all compute facilities → Condor + Globus V2

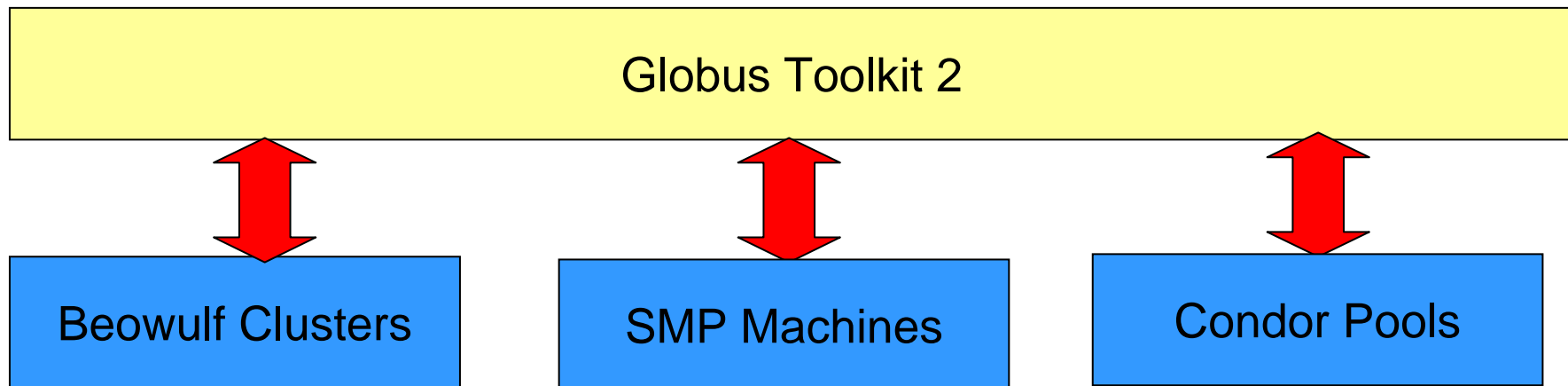
One File System – on all facilities – computing and data -> Storage Resource Broker (SDSC + CCLRC)

Metadata Capture for all activities – CML + CCLRC Scientific Metadata Model -> Metadata Editor

One Stop Data Access – to all data → CCLRC DataPortal Software

- **Sharing of resources using Globus Toolkit 2**

- Common security infrastructure
- Common access mechanisms
- Degree of abstraction from underlying system

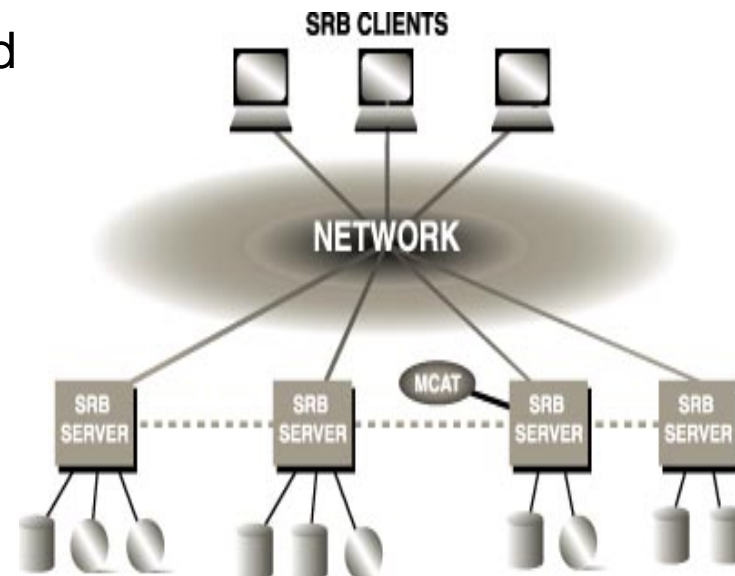


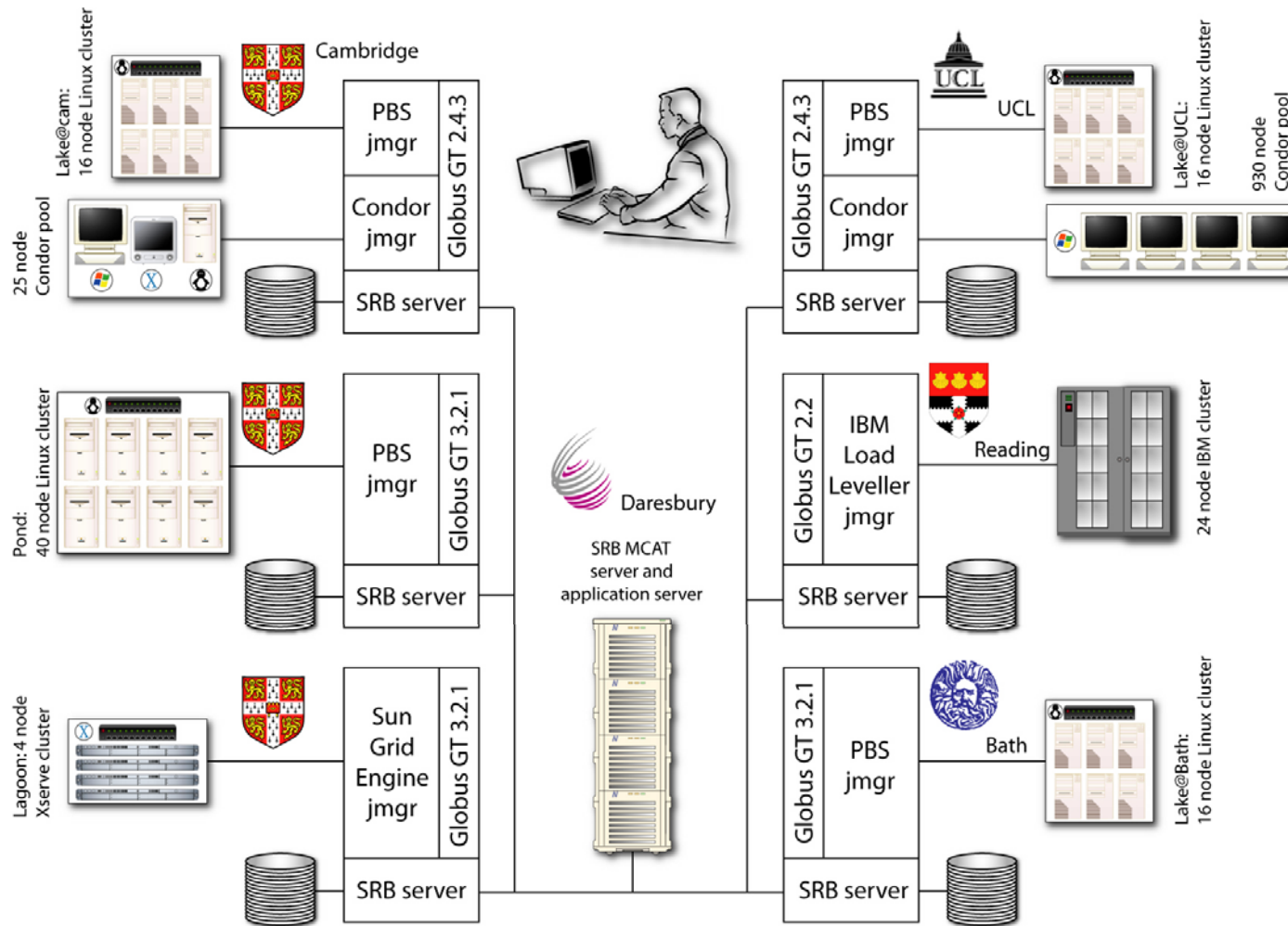
- **Aggregation of resources using Condor**

- Can build significant resources for HTPC out of existing infrastructure

- **Distributed file system using SRB**

- Files can be organised logically regardless of physical location and storage media
- Facilitates sharing of data files within VO and to collaborators
- Data files / executables are immed resources





Scientists are able to:

- **Put their input files into their SRB Directory**
- **Choose a suitable application executable in SRB**
- **Use the Condor DAGMan to define workflow/dependencies for calculation allowing for parameter sweeps, ensemble runs and linked execution**
- **Choose suitable resource type**
- **Submit DAGMan Script using their e-Science Certificate**
- **Review results in SRB**



open study

- Home
- Open
- View
- Admin

General details

Title chlorothalonil

Description Study by Helen HY Tsui PhD 2001 using anisotropic repulsion potentials. MR Tremayne et al, JACS submitted

More datasets to add? In Progress

Notes

Start date 20 October 2003

End date

Metadata created by /C=UK/O=eScience/OU=CLRC/L=DL/CN=lisa blanshard

On 20-OCT-2003 11:10

Investigators

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 Email: s.l.price@ucl.ac.uk Web: <http://www.chem.ucl.ac.uk/people/slprice/>

Dr DS Coombes
 RI, The Royal Institution of Great Britain, 21 Albemarle Street, , London, , W1S 4BS, UK
 Tel: +44 (0)20 7670 2934 Fax:
 Email: davidc@ri.ac.uk Web: <http://www.ri.ac.uk/DFRL/D.S.Coombes/publish/Home.html>

Dr LS Price
 UCL, University College London, Gower Street, , London, , WC1E 6BT, UK
 Tel: Fax:



Home
Open
New
Admin

change dataset details

chlorothalonil

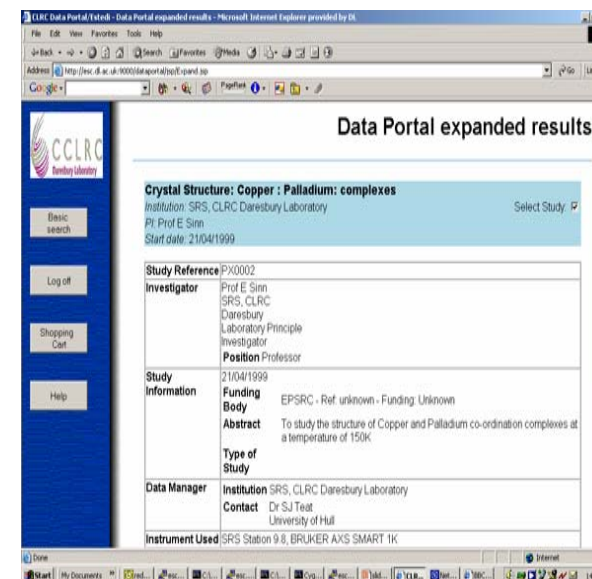
Dataset details (indicates a mandatory field)**

Name**	<input type="text" value="Low energy structure morphc"/>
Location of Dataset (URI)**	<input type="text" value="srb://eminerals.dl.ac.uk/home/sally_price.eminerals/c"/>
Description	<input type="text" value="Cerius generated morphologies using attachment energy model and FIT potential"/>
Status**	<input type="text" value="Complete"/>
Machine used**	<input type="text" value="helium"/>
Start date DD/MM/YY**	<input type="text" value="20/10/2003"/>
End date DD/MM/YY**	<input type="text" value="20/10/2003"/>

The CCLRC DataPortal

DataPortal – One stop shop to search for and access data from different organisations on heterogeneous systems in a uniform way. Allows parallel querying of various resources, offers personal permanent workspace to work with the data. The system is based on a web services architecture, connects well with other services and offers a high level of security.

<http://www.e-science.clrc.ac.uk/web/projects/dataportal>



Data Portal expanded results

Crystal Structure: Copper : Palladium: complexes Select Study

Institution: SRS, CLRC Daresbury Laboratory
PI: Prof E Srin
Start date: 21/04/1999

Study Reference	PX0002
Investigator	Prof E Srin SRS, CLRC Daresbury Laboratory Principle Investigator Position Professor
Study Information	21/04/1999
Funding Body	EPSRC - Ref unknown - Funding Unknown
Abstract	To study the structure of Copper and Palladium co-ordination complexes at a temperature of 150K
Type of Study	
Data Manager	Institution SRS, CLRC Daresbury Laboratory Contact Dr SJ Teat University of Hull
Instrument Used	SRS Station 9.8, BRUKER AXS SMART 1K

Microsoft Internet Explorer browser interface showing the address bar with the URL <http://ematerials.cclrc.ac.uk:8080/dataportal/jsp/SimpleSearch.jsp> and various navigation icons.

Start date: 2003-10-17 00:00:00.0

6

Polymorph prediction of aspirin

Institution: UCL

Select Study:

PI: Sally SL Price

Start date: 2003-10-14 00:00:00.0

kflds;ajfkaj

chlorothalonil

Institution: UCL

Select Study:

PI: Sally SL Price

Start date: 2003-10-20 00:00:00.0

Study by Helen HY Tsui PhD 2001 using anisotropic repulsion potentials. MR Tremayne et al, JACS submitted

Expand selected results





Shopping Cart

Home > Basic Search > Studies > Expanded Studies > Data > Shopping Cart

DataSet	Notes	Resend Query	Transfer	Date added		Delete
fiddle	View	Ok	transfer	Mon Oct 20 12:56:13 BST 2003	n/a	<input type="checkbox"/>
Low energy structure morphology data	View	Ok	transfer	Mon Oct 20 17:02:32 BST 2003	n/a	<input type="checkbox"/>
Webpages	View	Ok	transfer	Mon Oct 20 12:32:54 BST 2003	n/a	<input type="checkbox"/>
work	View	Ok	transfer	Mon Oct 20 12:45:50 BST 2003	n/a	<input type="checkbox"/>

- Home
- Basic Search
- Shopping Cart
- user
- History
- log out
- Information
- Help
- Documentation
- Data Portal
- e-Materials

Date [v] Sort [v] Delete all c [v]

Notes - Microsoft Internet Explorer

Low energy structure morphology data
 Study: chlorothalonil
Initial Query:
 Facility(s): EMAT
 Discipline: /Chemistry/Computational/Solid State/Organic/Crystal Structure Prediction/Aspirin
 Waiting time: 15 seconds

Delete



Edit View Favorites Tools Help

Back Search Favorites Media Link

Address: http://ematerials.cclrc.ac.uk:8080/dataportal/jsp/srb.jsp?url=srb://ematerials.dl.ac.uk/home/sally_price.ematerials/chlorothalonil/low_energy_structures/morphology Go

Search Web Search Site PageRank Options



SRB Download

Home > Basic Search > Studies > Expanded Studies > Data > Shopping Cart > SRB transfer

Name of collection to srb://ematerials.dl.ac.uk/home/sally_price.ematerials/chlorothalonil/low_energy_structures/morphology transfer :

Url of destination :

WinZip (Unregistered) - morphology[1].tar

File Actions Options Help

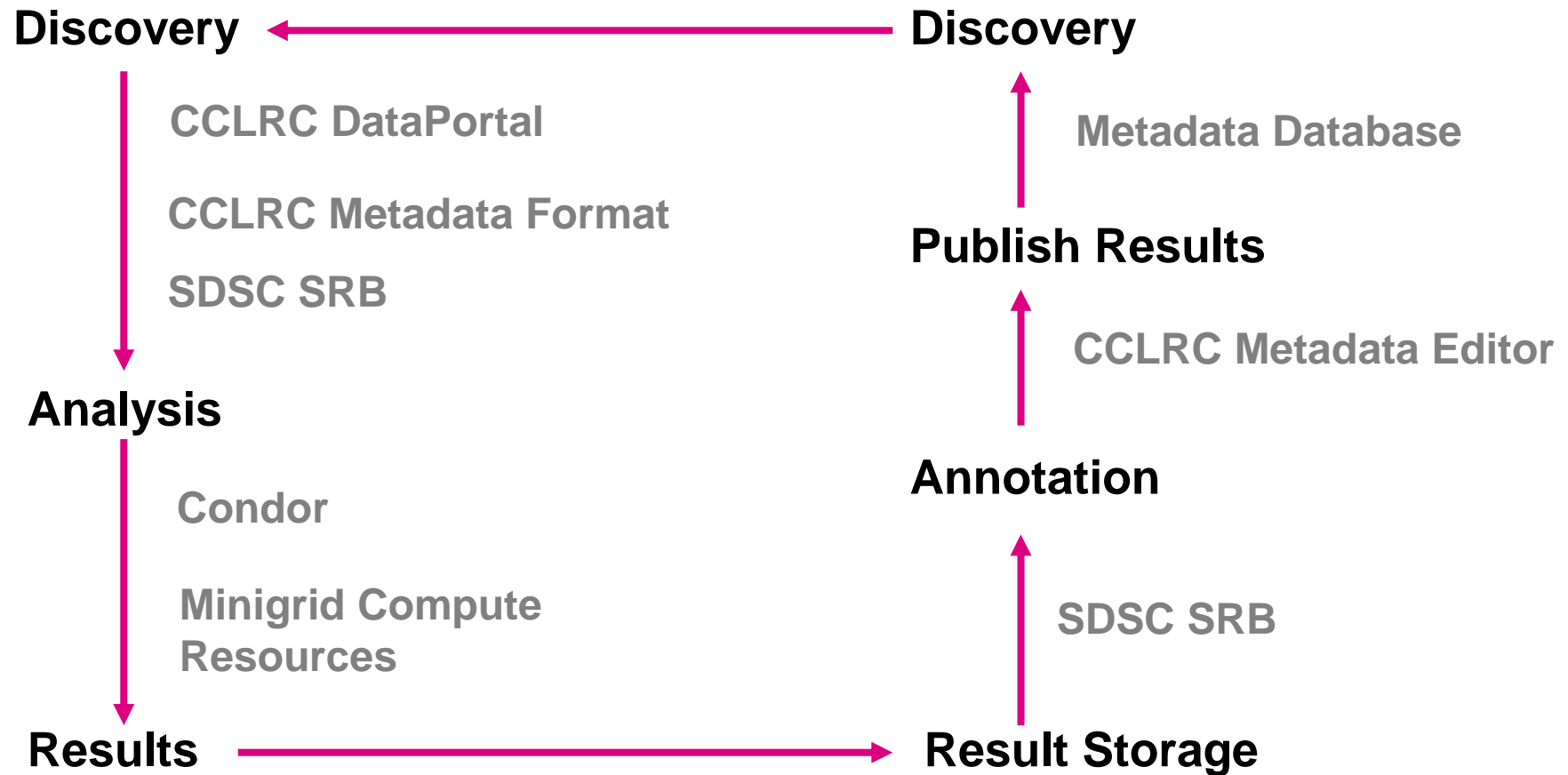
New Open Favorites Add Extract View CheckOut Wizard

Name	Type	Modified
AB11f.dat.gz	WinZip File	21/10/2003 1...
AB11f.hab.gz	WinZip File	21/10/2003 1...
AB11f.inf.gz	WinZip File	21/10/2003 1...
AB11fi.rgb.gz	WinZip File	21/10/2003 1...
AB15f.dat.gz	WinZip File	21/10/2003 1...
AB15f.hab.gz	WinZip File	21/10/2003 1...
AB15f.inf.gz	WinZip File	21/10/2003 1...
AB15fi.rgb.gz	WinZip File	21/10/2003 1...
AB25f.dat.gz	WinZip File	21/10/2003 1...
AB25f.hab.qz	WinZip File	21/10/2003 1...

Selected 0 files, 0 bytes Total 84 files, 444KB

- Home
- Basic Search
- Shopping Cart
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- History
- Log out
- Information
- Help
- Documentation
- Data Portal
- e-Materials





Automation of Metadata Capturing Processes

Linkage to e-Publication

Better Search Interfaces

Virtual Dataset Generation + Annotation Facilities

**Assimilation and Mining of Data from variable
Sources**

- **Have production minigrid infrastructure comprising data, metadata, HPC and HTPC resources**
- **Minigrid infrastructure has enabled real science research**
- **Working on further integration of different areas of functionality within minigrid**

Thank you for you attention.

Any questions??

Contact details

<http://www.e-science.clrc.ac.uk>

k.kleese@dl.ac.uk
