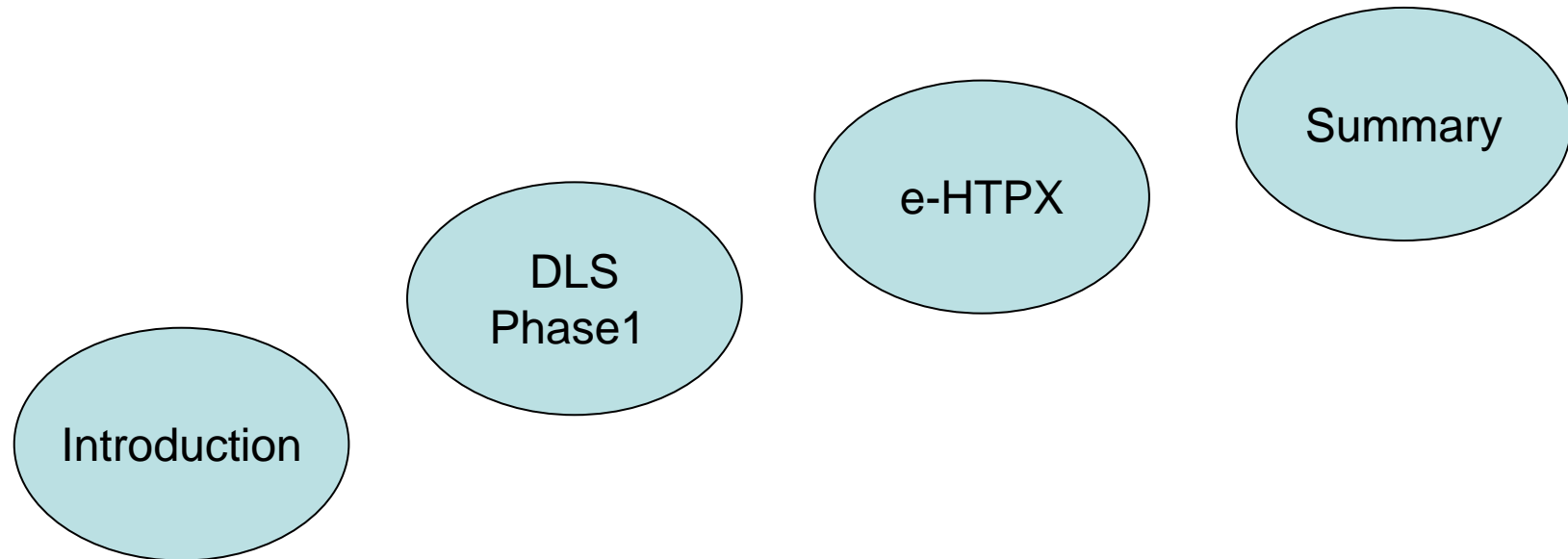


# Integrating macromolecular crystallography into the Generic Facilities Data Management

Michael Gleaves

# Outline



# Introduction

The Phase 1 development work for DLS focused on:

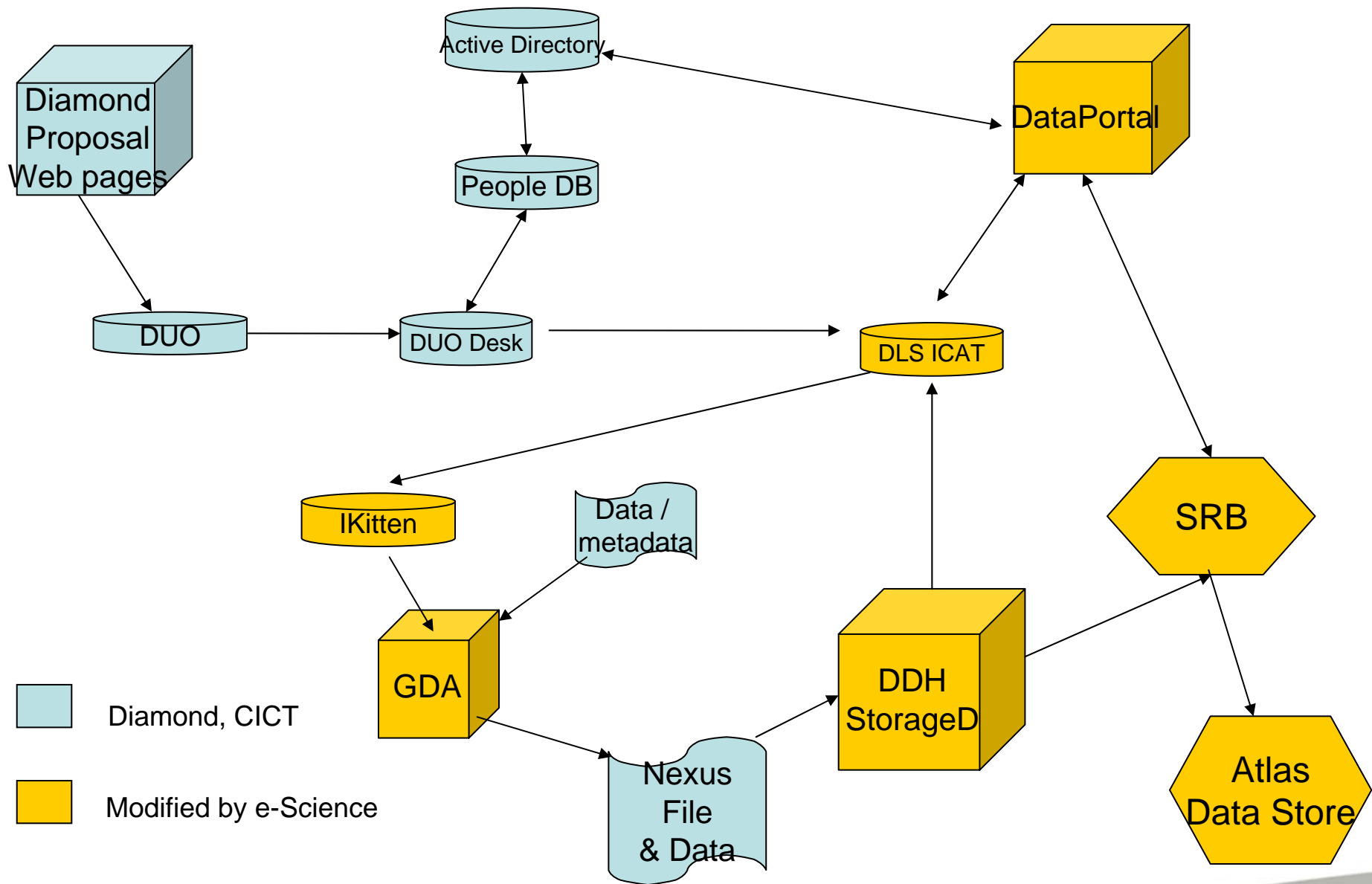
- Single Sign On applied to all modules.
- Integration of the GDA (Generic Data Acquisition) to the e-Science framework.
- Automatic collection of metadata relating to the experiment.
- Storing the raw data in the ATLAS data store for long term data management.
- View and retrieve data.

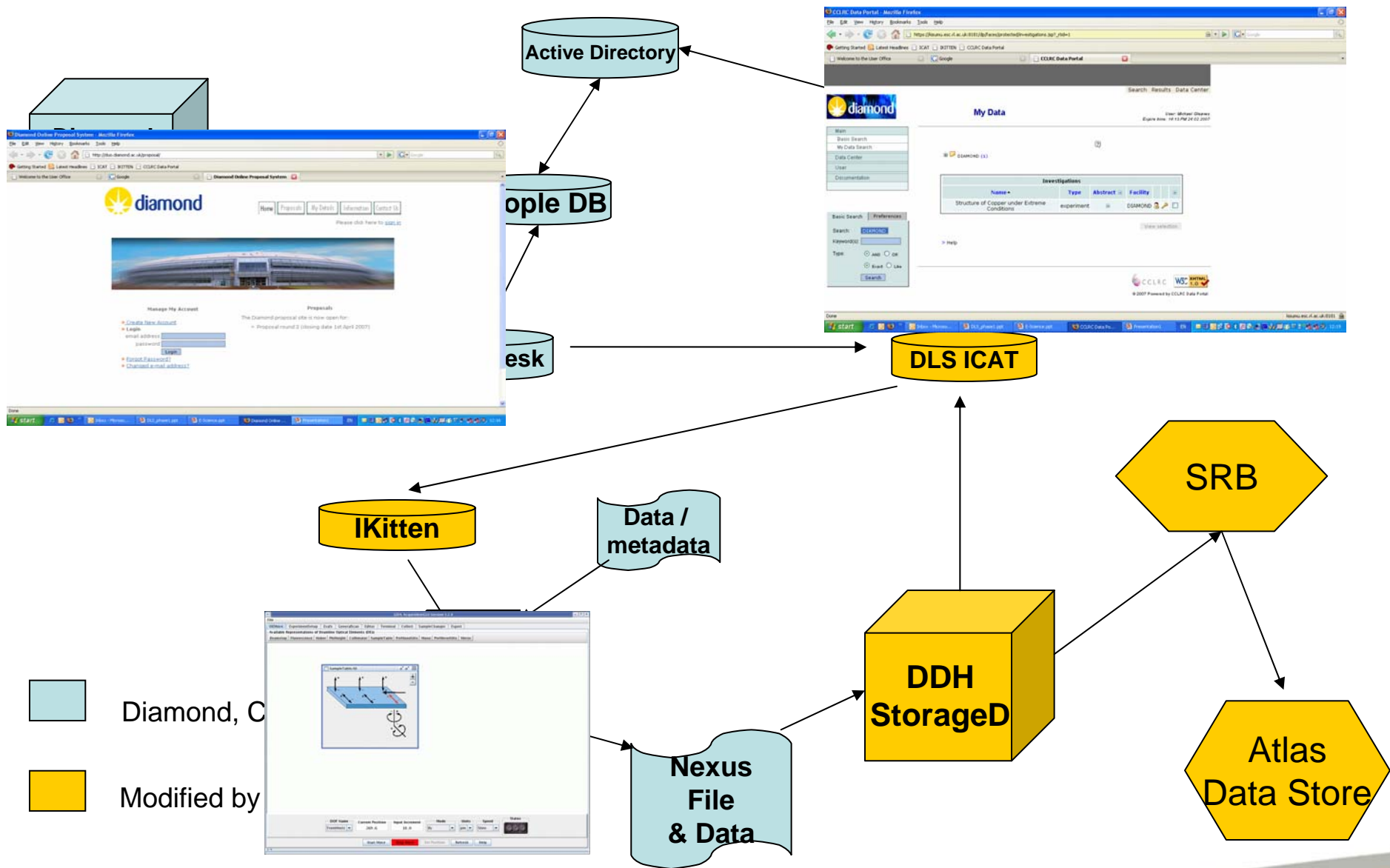


# Design Rules

1. Must fit in with existing tools GDA – web based proposal system.
2. Relies on the only the beamline network.
3. Should never prevent data collection.





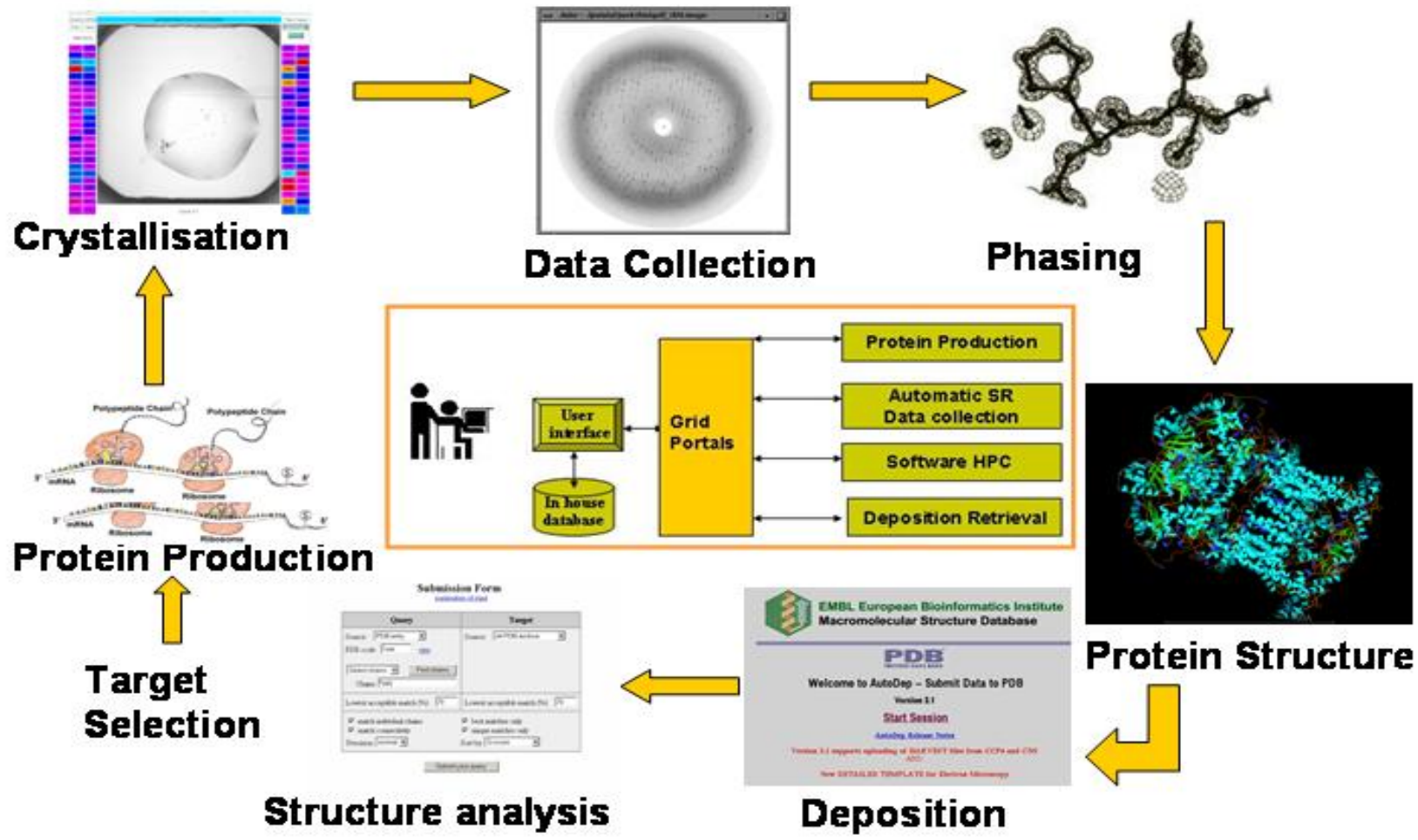


# e-HTPX

BBSRC funded project to unify the procedures of protein structure determination into a single all encompassing interface from which users can initiate, plan, direct and document their experiment either locally or remotely from a desktop machine.



# Overview of Protein Crystallography





# Outputs of e-HTPX

- e-HTPX messaging model (XML schema that describes the information transferred between web service)
- Portals that are the interface designed in conjunction with Protein Crystallographers
- Both York structural Biology lab and OPPF are using this to manage their trips to ESRF BM14.

The screenshot displays the e-HTPX Portal interface. The main content area is titled "View Shipment - OPPF - BM14". It includes a "Details" section with a table of shipment information:

Reference Date	Reference	From	To	Description	Contact User	Authorized By	Authorized Date	Shipped Date	Arrival Date
17052206	oppf1	OPPF	BM14		ian@stxuk.es.ac.uk	ian	17052206	17052206	17052206

Below the table is a "Shipping Agent" table:

Shipping Agent	Agent ID	Flight Code	Shipping Date	Delivery Date	Edit
Karl Hansen Cruisers	007	B457	17052206	17052206	Edit

The interface also shows a "History" section with a table of events:

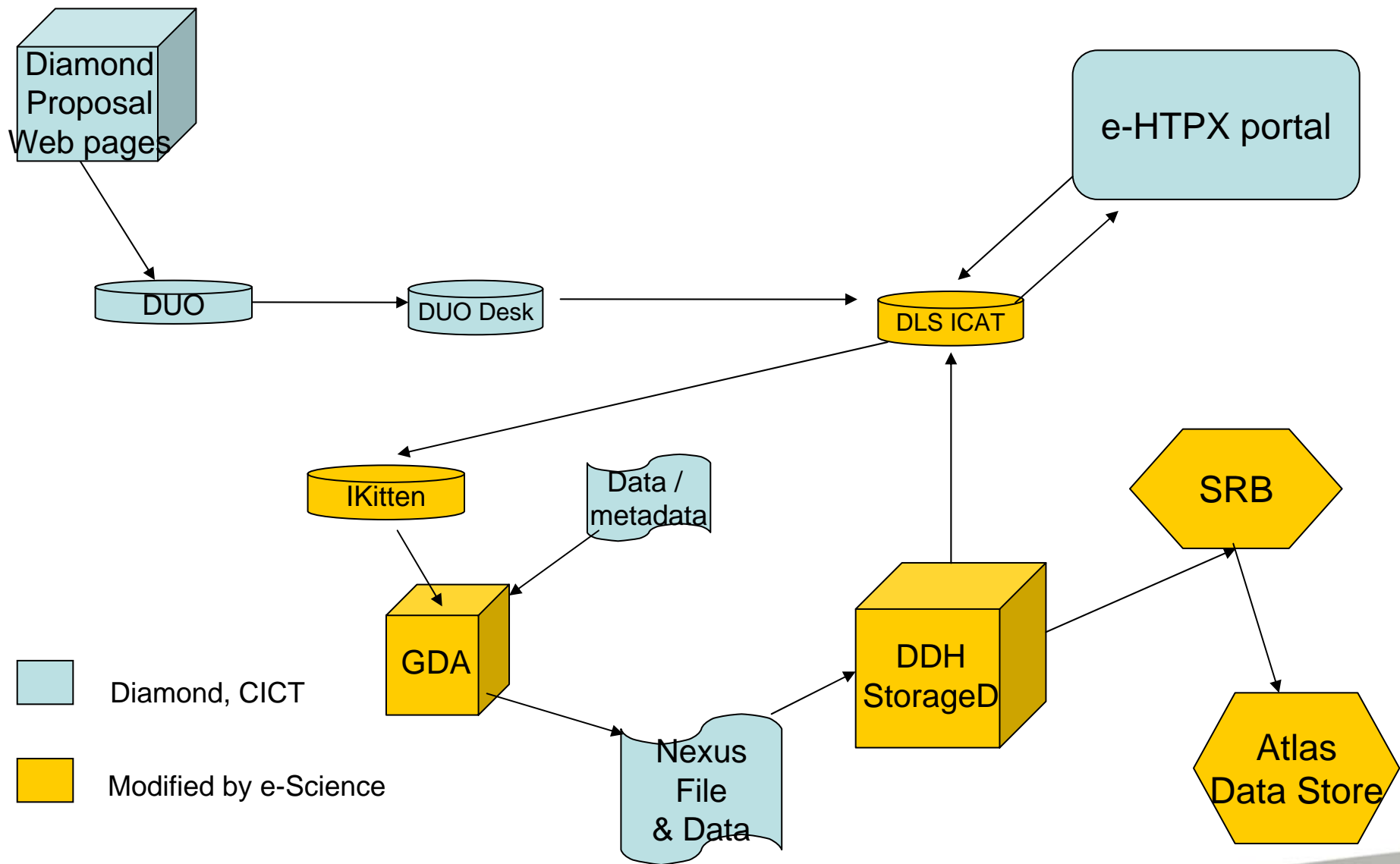
Event Type	To Date	Amount
May 17, 2006	May 17, 2006	0.000
May 17, 2006		BM14

At the bottom, there are sections for "Current Subcontainers" and "Subcontainers". The "Current Subcontainers" table lists:

Event Name	Name	Barcode	Description	View
OrdShip1	OrdShip1	OrdShip1	The one with the rest lol	View
OrdShip1	OrdShip1	OrdShip1	OrdShip1	View

The "Subcontainers" section shows two panels: "Other Subcontainers" and "Current Subcontainers". The "Current Subcontainers" panel lists:

- Igl00: OrdShip1
- Segment Dewar: OrdShip1



# Summary

Planning to manage data for users on a facility level.

Add value in making post analytical codes available

Integration of domain specific portals

## Any questions?

# Acknowledgements

**DLS people** – Alun Ashton, Stuart Campbell, Bill Pulford.

**DL SciTech-** Rob Allen, Karen Ackroyd, Lisa Blanshard, Phil Couch, Glen Drinkwater, Roger Downing, Steve Kinder Shoaib Sufi, Rik Tyer.

**DL e-HTPX** – Colin Nave, Dave Meredith, Ronan Keegan, Graeme Winter.