

Database Requirements for CCP4 Projects

Monday 17th October 2005

Abstract

- Gather information on the current and future needs and concerns of CCP4-related projects with regard to data management and the use of databases within CCP4 for structure determination
- i.e. what are the database requirements for CCP4?

Issues to be considered:

- what are the data being stored?
- what are the needs for data models?
- consideration of possible database technologies

This meeting will not resolve these issues – it is a starting point for discussion and to decide steps needed to progress

Questions:

- What sort of "database(s)" do you want/need/use now in your project e.g. databases of structures, ligands etc.
- Do you want to be able to track operations that the user might perform (and if so at what level)?
(Tracking means keeping a record of what has been done in order to visualise, backtrack, restart etc.)
- Do you want to store crystallographic data in it? Do you want to retrieve crystallographic data from other applications from it? What data in particular?
- Are there any technical issues, e.g. preferred languages for APIs?
- What do we already have that we can use now?

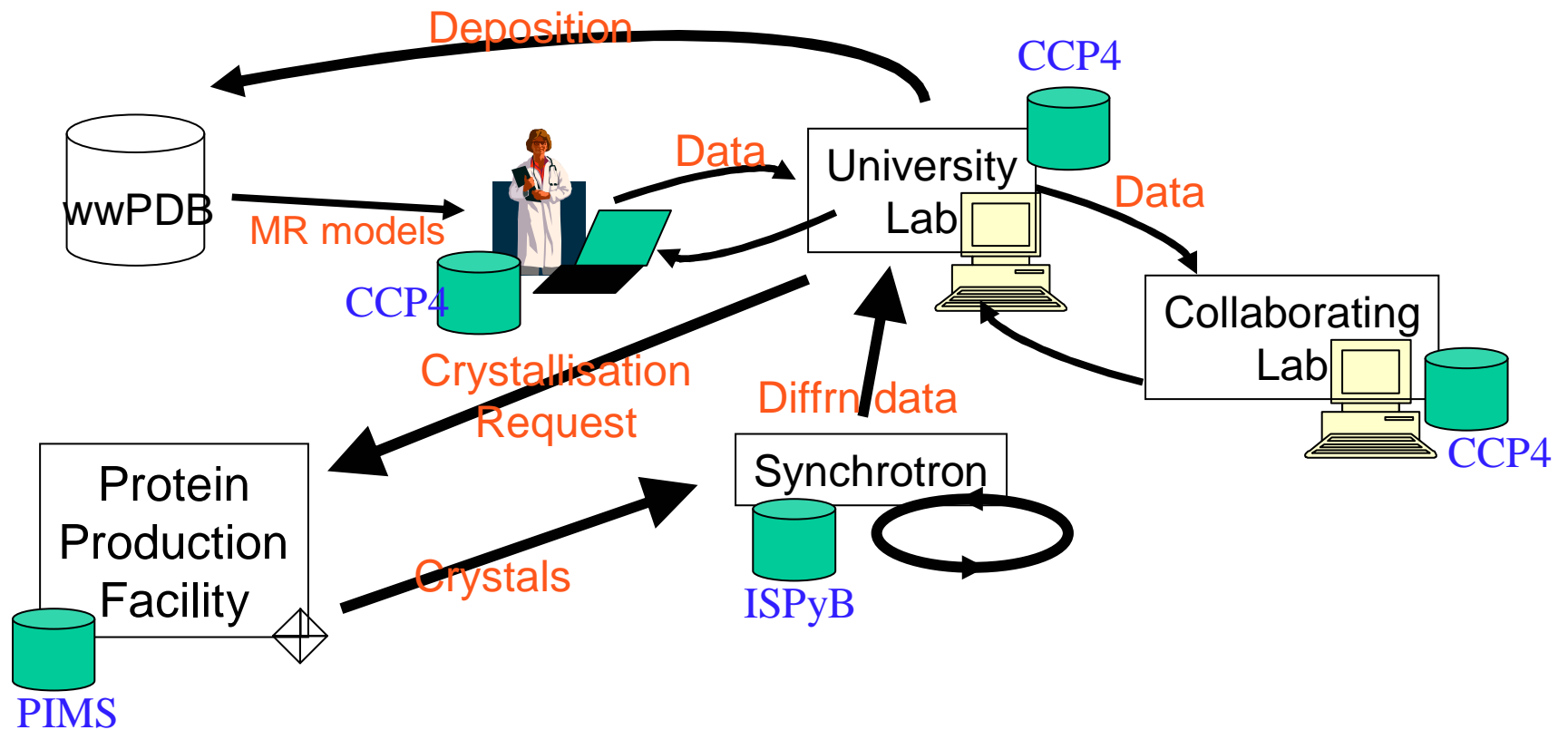
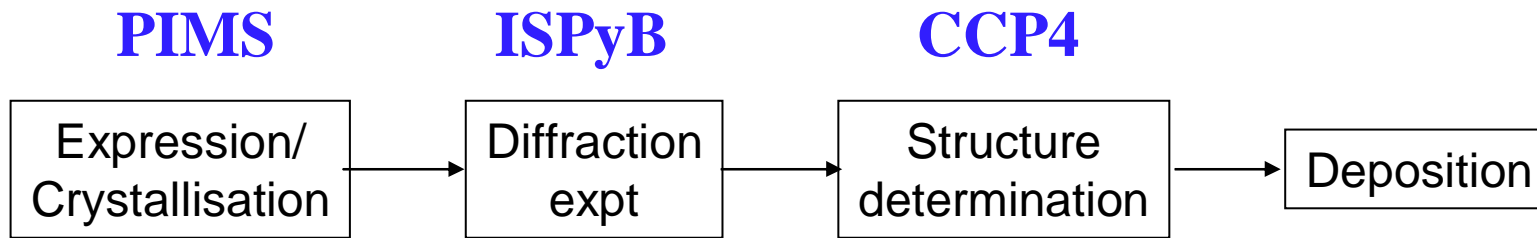
DL DB Meeting: PIMS, ISPyB, e-HTPX, CCP4/BIOXHIT

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Examined scope and interfaces/overlaps/data exchange issues between these projects:

- PIMS: expression/crystallisation
- ISPyB: beamline/data collection
- CCP4/BIOXHIT: post data collection
- e-HTPX: glue to hold these together

- Interface between PIMS & ISPyB
 - ongoing issue to be resolved within e-HTPX
- ISPyB “wraps” DNA on beamlines
 - stops after storing screening results & images
 - ESRF may wish to extend this in future
 - GW using prototype CCP4 db for data processing
 - implementation on beamlines is political issue
 - action to look at this
 - pipeline between ISPyB/DNA & CCP4 db in home lab is a gap
- Location of databases also an issue
 - e.g. ISPyB at the home lab, CCP4 db on beamlines
 - requirement to export/import data to move around



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Time	Talk	Speaker
10:20	Welcome and introduction	
10:30	Data modelling: some lessons from experience <i>plus discussion</i>	Chris Morris
11:30	CCP4(i)/Bioxhit Database Project	Peter Briggs
12:00	Lunch	
13:00	CCP4 Automation	Charles Ballard
13:30	e-HTPX	Graeme Winter
14:00	York Refmac/Molrep pipeline	Garib Murshudov
14:30	CRANK	Steven Ness
15:00	Coffee break	
15:30	CCP4i	Peter Briggs
15:40	CCP4mg	Liz Potterton
15:50	Coot	Paul Emsley
16:00	Discussion: contents of DB for automation of structure solution using existing knowledge and information	Chaired by Garib Murshudov
17:00	Close	

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