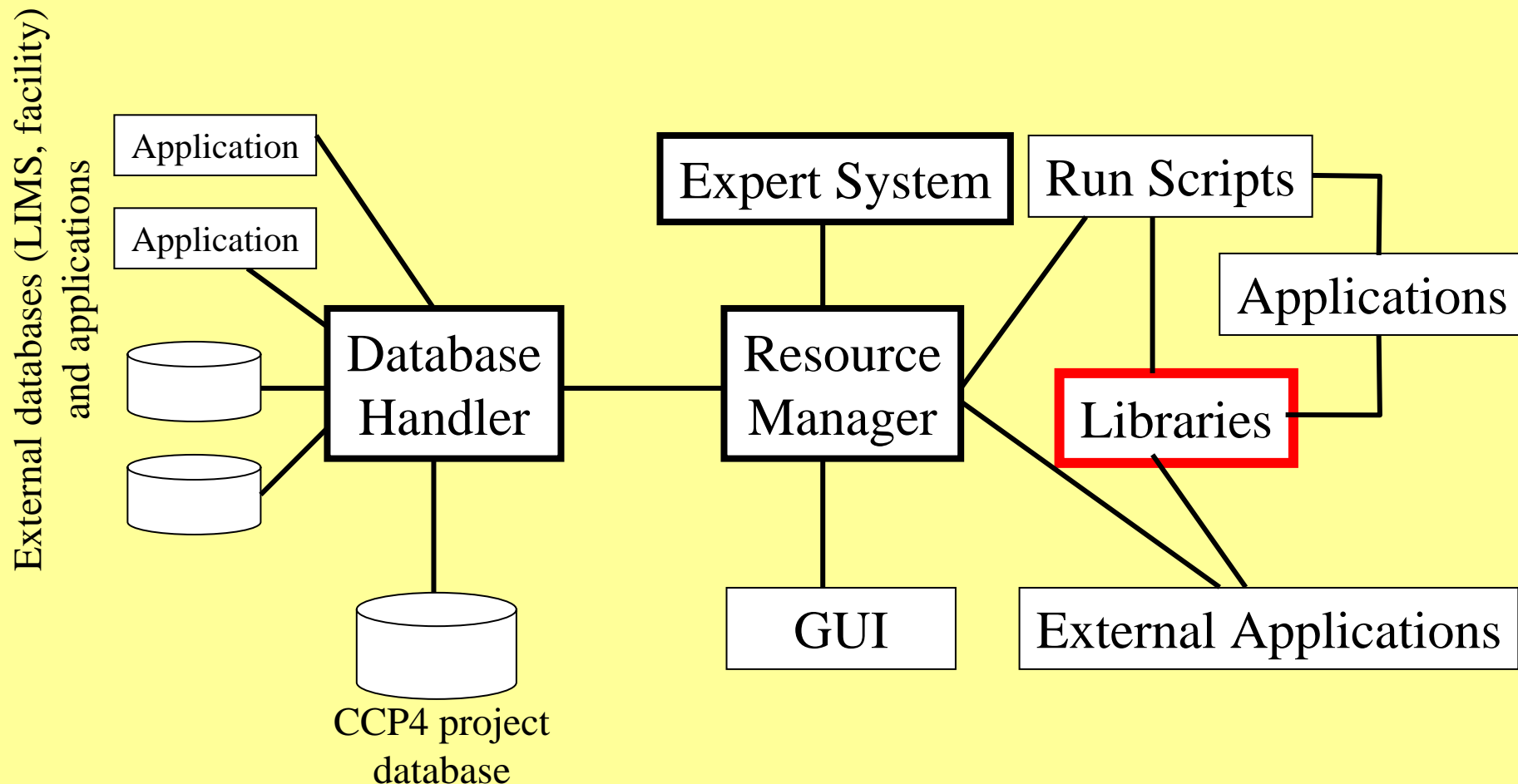


Task 4.7.1:
Automation in Computation

Peter Briggs, CCP4

Context: CCP4 Developments towards Automation

- Core library developments
- Provision of “unified environment for general automation and rapid development of new applications”
- CCP4 Automation Project
 - Starting soon



Recently CCP4 have been engaged in re-implementing the core software libraries:

- Low-level functions (file handling, symmetry etc)

Aims:

- Implement better description of the underlying data models
- Provide support for C/C++/scripting languages
- Maintain support for existing programs

The next stage is provision of a “PX software toolbox”

PX toolbox: Aims

- Identify useful “medium-level” functionality:
 - e.g. sorting/merging of reflection data, FFT generation
 - within existing “computational units” (i.e. programs)
 - currently missing from the suite
- Abstract these functions into a library (“toolbox”)
 - can be exploited directly from within programs/scripts
- Provide interfaces to the functions for a number of programming/scripting languages

PX toolbox: outcomes

- Rapid development e.g. via scripting (Phenix model)
- Fill a (perceived) gap below the level of complexity of systems like Clipper
- Feed into
 - BIOXHIT structure solution software pipelines
 - CCP4 Software Automation Project
 - other projects?

Within context of BIOXHIT:

- Early stages (within first 12 months):
Liaise with BIOXHIT Partners to determine requirements and specification for toolbox functionality, choice of programming languages etc
(Some overlap with WP5.1?)

***Report on evaluation/identification of functions
(deliverable 4.7.1) will inform development of toolbox***

- Later stages:
Transfer developments to BIOXHIT Partners