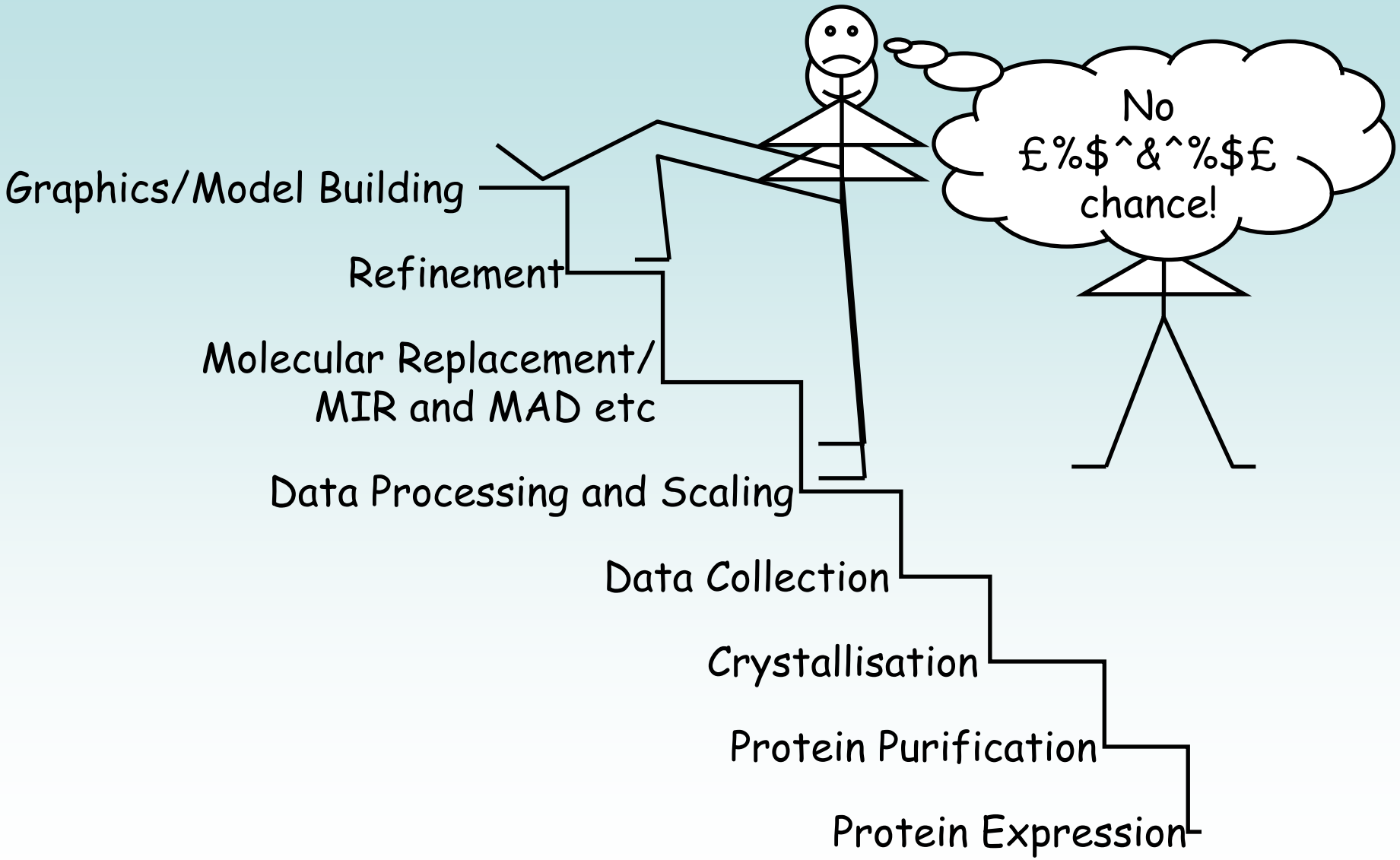
MOLE

- A Laboratory Information Management System specialising in tracking the progress of targets through structure determination.
- Utilising free and commonly available software.
- Based on internationally accepted, cross discipline data models.
- Released and supported the CCP4 way.

You don’t care do you?


No
£%$^&^%$£
chance!
Graphics/Model Building
Refinement
Molecular Replacement/
MIR and MAD etc
Data Processing and Scaling
Data Collection
Crystallisation
Protein Purification
Protein Expression

The CCP4i Experience

(Current status – See Pete for future plans!)

5.0.f CCP4Interface 1.3.15 running on CCP4PORT1 Project: ascamr2

running) in this project

Help

11	02 Jan 00	FINISHED	dictionary	ttq regula
10	28 Jul 03	FINISHED	beast	find 2nd m
9	28 Jul 03	FINISHED	beast	refine rot
8	28 Jul 03	FINISHED	beast	[No title
7	28 Jul 03	FINISHED	molrep	[No title
6	28 Jul 03	FINISHED	molrep	[No title
5	28 Jul 03	FINISHED	mr_solution	Build mode
4	28 Jul 03	FINISHED	amore	refine ste
3	28 Jul 03	FINISHED	amore	translatio
1	28 Jul 03	FINISHED	matthews	

Directories&ProjectDir

View Any File

View Files from Job

Delete/Archive Files..

Kill Job

ReRun Job..

List of jobs (finished or running) in this project

CCP4Interface 1.3.15 Directories & Project Directory

Enter one-word alias and full directory path for your Project directory(s).

Deleting these project definitions will not delete the actual directories.

Project PROJECT uses directory: C:/WINDOWS/Temp

Project ascamr uses directory: C:/awa/mrtut

Project ascamr2 uses directory: C:/awa/mrtut/f/GUI2

Project new uses directory: C:/awa/mrtut/f/new/GUI

Edit list Add

Project for this session of CCP4Interface ascamr2

Enter one-word alias and full directory path for other directories you use regularly.

Alias: TEMPORARY for directory: C:/WINDOWS/Temp

Alias: example for directory: C:/CCP4win4_2_2a/examples/rnase

Alias: fdata for directory: C:/awa/mrtut/f

Alias: map for directory: C:/CCP4win4_2_2a/html/AstexViewer_man

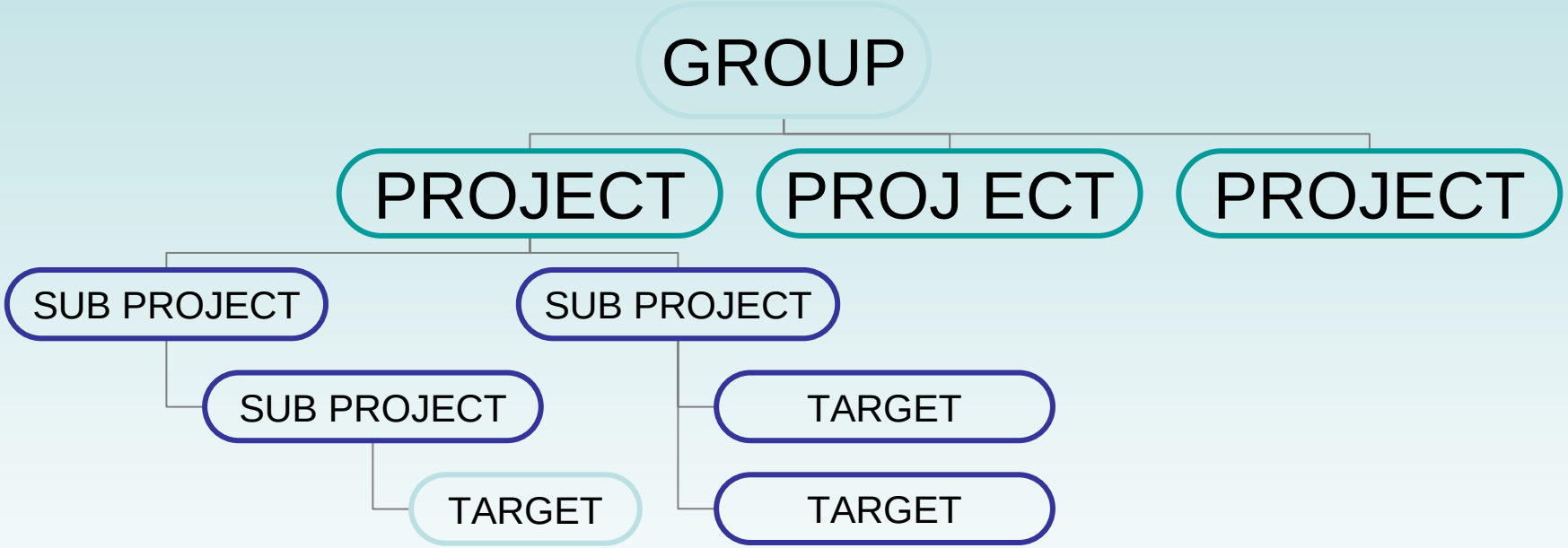
Edit list Add directo

Data stored in ASCII files.

MOLE the pilot project.

- Started Coding October 2002
- Web interface
- Should not be tied to any particular DB
- Easy to install
- Easy to support
- No propriety tools
- Based on the Data Model
- Secure
- Flexible / customisable
- Easy and desirable to use.

Groups in MOLE



Security.

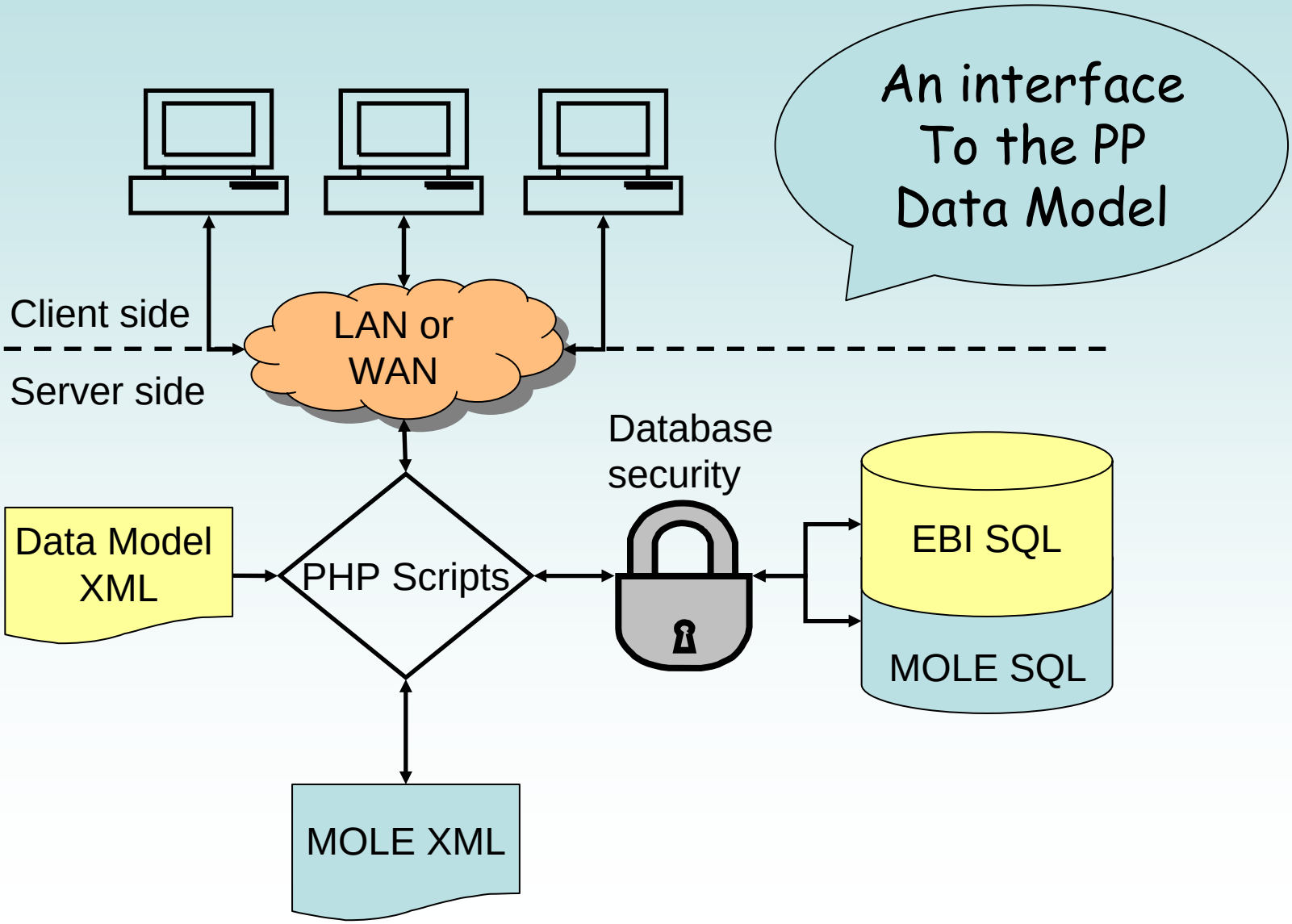
- Security can be intranet
- Security can be https
- Security can be Database / Group
- Security can be table

- Security should not be at the application layer – but the application should be secure and not expose the data!

The Protein Production Data Model

- An EBI/eHTPX initiative to standardise and describe the data items required to record and reproduce experiments.
  - Protein Production data items described in mmCIF
  - UML data model produced to describe relationship between PP data items
- UML translated for application programmers
  - SQL and XML representations (EBI)
  - Source code API (CCPN)
- Current Version 0.9.6
  - Versions first available March'03

MOLE V0.2.0 released FEB'04



MOLE

Login/Security

Please login:

User Name:

Password:

Login

Database Level Security
(https could be extra level)

Projects

Project/Group Information

Group: mole_demo Parent Project: Photosynthetic Proteins Change Group:

Projects	Contents...
Reaction Centre	YM177F
	NATIVE
	RM197F
Light Harvesting Complex	

User defined
Group/Project
Hierarchy

Admin

Edit User

Edit Existing User:

CCP4 User's Information:

User admin tools

Install Setup

Initialise MOLE DB Setup:

System Information:

Backup Information

SQL install/backup

MOLE Installation Setup

Edit Configuration Options :

XML configuration file
Including DB choice,
Language…..

Central Server
Apache/PHP/RDBMS

Interfaces

MOLE

Hello CCP4! Welcome to MOLE v0.01

MOLE - mining organising and logging experiments

Targets/Tracking

Your Default Target:

Group: PUBLIC - Project : Reaction Centre [Rotate 90]

Target: 7 - YM177F

CULTURE → LYSIS → FRACTIONATION → FRACTIONATION → CHRO → CHRO

Start New Experiment Path

Key: TO DO OK IN PROCESS FAILED

Database driven views

Daresbury Lab LIMS [Experiments] - Microsoft Internet Explorer

Characterisation Experiments	Help	Further Help
CHARACTERISATION	[Help]	More...
CIRCULAR_DICHROISM		More...
DYNAMIC_LIGHT_SCATTERING		More...
GEL_ELECTROPHORESIS	[Help]	More...
MASS_SPECTROSCOPY		More...
NMR		M
OPTICAL_DENSITY_TIME_SERIES		
SEQUENCING		

Protein Production Experiments	Help
CELL_FREE_EXPRESSION	[Help]
CHROMATOGRAPHY	[Help]
CONCENTRATION	
CULTURE	
DIGEST	[Help]
DISH_CULTURE	[Help]
DNA_PURIFICATION	
EXPRESSION	[Help]
FRACTIONATION	[Help]
LIGATION	[Help]
LYSIS	[Help]
MINIPREP	[Help]
PCR	[Help]
PROTEIN_PURIFICATION	
PROTEOLYSIS	[Help]
RECOMBINATION	[Help]
REFOLD	[Help]
TRANSFORMATION	

Experiments/Help

Experimental Information

PPRO_CHROMATOGRAPHY (11 of 13)

PPRO_CHROMATOGRAPHY (Target:3)

Microsoft Internet Explorer

The yield in milligrammes of protein recovered in the pooled fractions.

OK

Data Model
XML derived help

CCP4

CCLRC
Daresbury Laboratory

Version 0.3.0 APR'04

- Code migration to allow multiple 'skins'
  - Different output formats
  - More complete language support
- Code migration to allow full security compliance
- Usability improvements

Beyond APR'04

- Project evaluation, design and consultation
  - Resource and partner evaluation
  - Technology evaluation and consultation
  - Timescales reset

- Continued prototype improvements
  - Sadly the user wants something now.

MOLE the CCP4 way….

- Full CVS repository
- Bugzilla feature tracking
- Helpdesk mole@dl.ac.uk
- Website www.mole.ac.uk
- Fairly up to date pdf manual

Thanks

- Chris
- Susy
- Data modellers
- Peter Wood…..

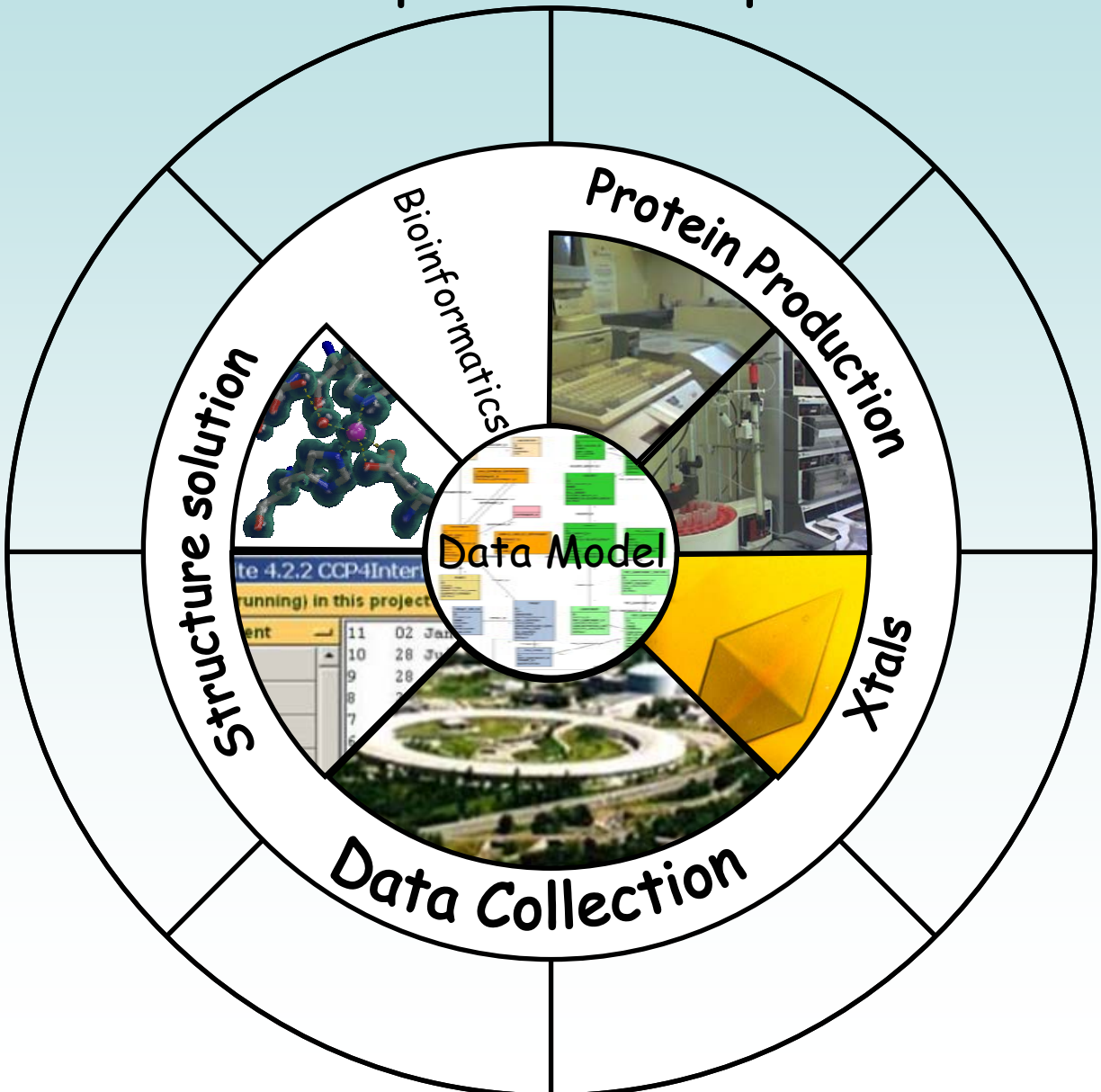
What about everyone else?

Relationship with other CCP4 projects

- CCP4i
- Crystal imaging
- Data collection

LIMGRID

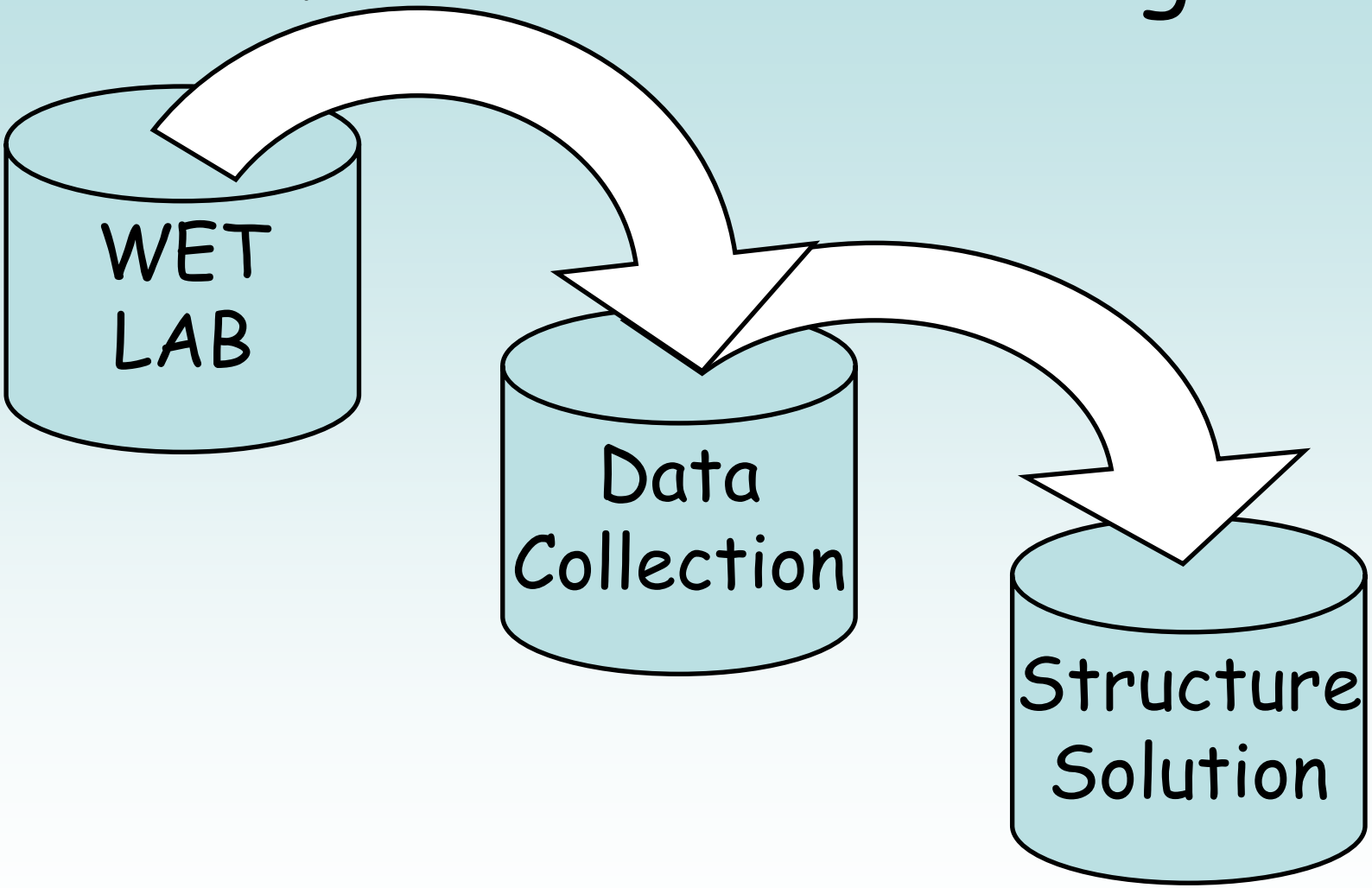
http://www.ccp4.ac.uk/LIMGRID



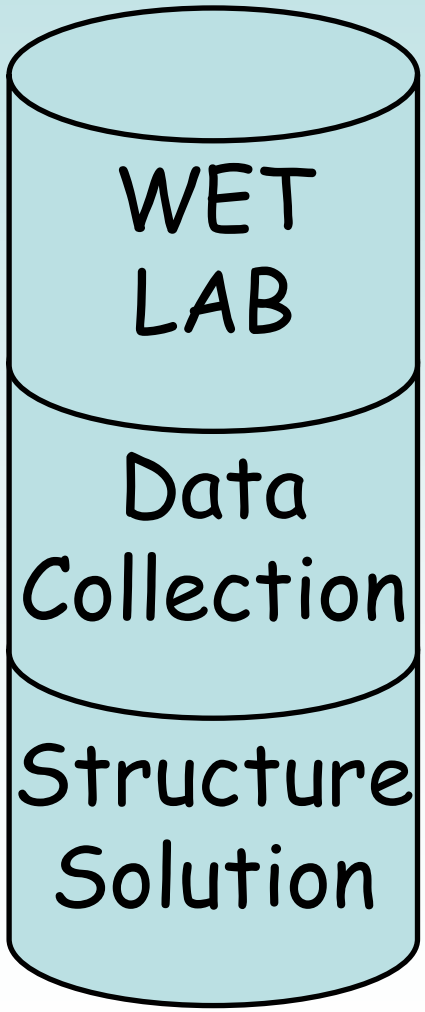
Partners include:

- MOLE
- ESRF
- CCP4
- EBI
- Daresbury Lab
- University of York
- eHTPX
- Oxford Protein Production Facility
- EMBL-Grenoble

Information Tracking.



Information Tracking.



"Trial"

Crystal ID

CrystalID
+ Data set