Projects

MMDB (*2000-2003*)

Description:	CCP4 Coordinate Library, support of coordinate-related functionality in protein crystallography applications, small molecules database (dictionaries).
Status:	***Generally completed***. Maintenance, support and further development as needs arise.
Availability:	CCP4 Release 5 Part 0 software
URL:	http://www.ebi.ac.uk/~keb/cldoc
Publications:	1. Software Practice and Experience - in print 2. Acta Cryst D. - submitted
Related projects:	1. CCP4 Molecular Graphics 2. CCP4 Molecular Building 3. Clipper 4. Parts of EBI-MSD deposition site 5. Parts of EBI-MSD ligand and active site services 6. Used by various developers world-wide (confirmed by feedback) 7. Potentially useful for any coordinate-related development: REFMAC, MOLREP and others.

Projects

SSM (*2001-2003*)

Description:	Comparison and alignment of protein structures in 3D, MSD-CCP4 web server / standalone application.
Status:	***Generally completed***. Anticipated development: a) closer integration with MSD database and possibly SCOP b) matching short fragments. Maintenance, support and further development as needs arise.
Availability:	Web-server, binary distribution from EMBL-EM under academic and commercial licences. SSM core algorithm to be distributed as source code under LGPL-compatible licence. Possible inclusion into later CCP4 releases as a standalone application.
URL:	http://www.ebi.ac.uk/msd-srv/ssm
Publications:	1. Software Practice and Experience - in print 2. Acta Cryst D. - submitted
Related projects:	1. CCP4 Molecular Graphics 2. CCP4 Molecular Building 3. Structural similarity in EBI-MSD database 4. Parts of EBI-MSD structural motif service 5. Used by SCOP 6. Used by researches world-wide (3200 unique URLs, 20,000 queries, 77 distributions for in-house installation)

Projects

Protein interfaces (2004-)

Description: Tools for chemical-topological analysis of protein surfaces and structures.

Status: ***Initiated***, under development.

Deliverables: Library of functional procedures, standalone applications, integrating Web-server, database of protein interfaces with tools for similarity queries

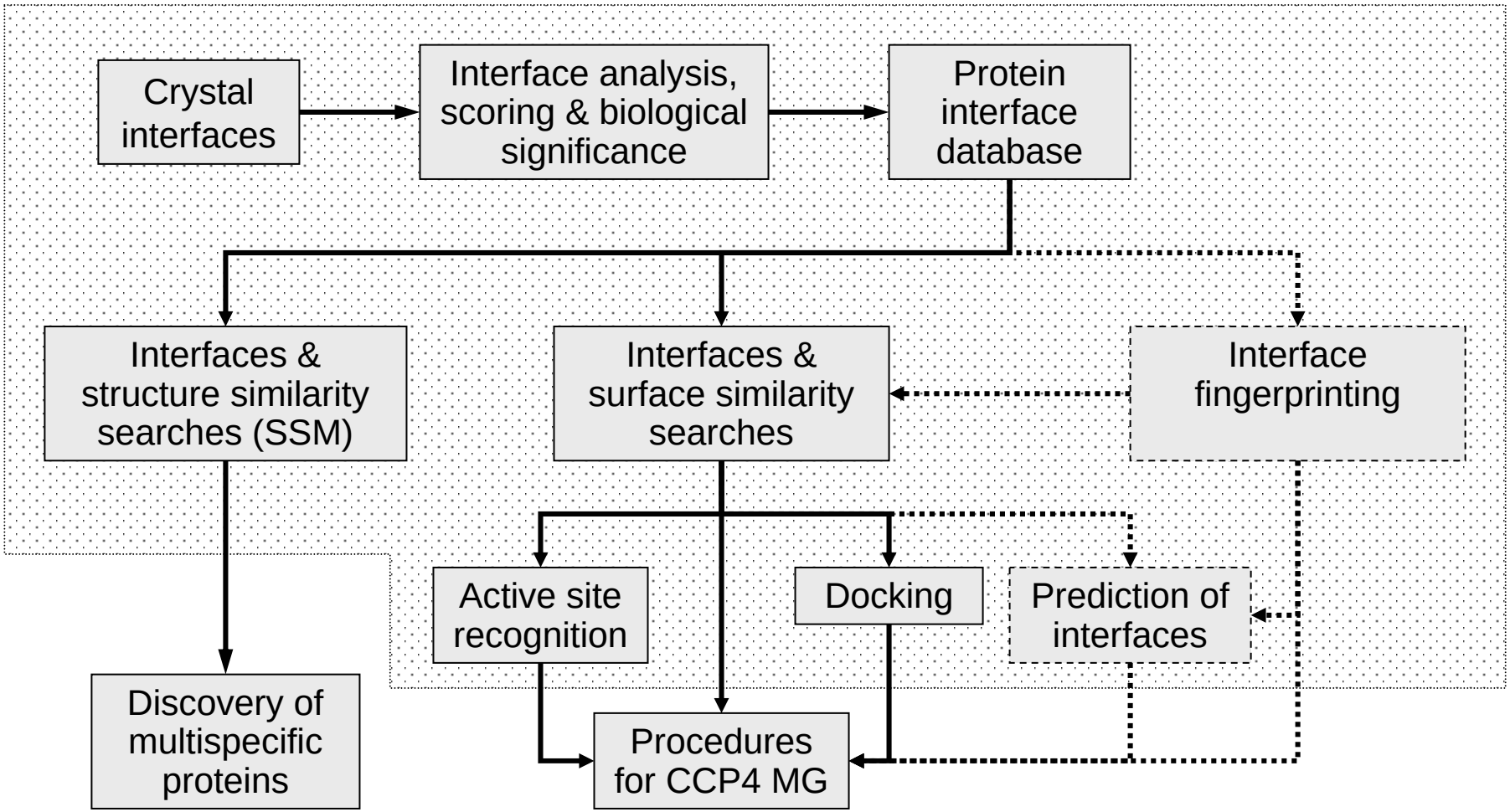
Potentially useful for:

1. CCP4 Molecular Graphics (surface analysis/matching, docking).
2. EBI-MSD database
3. Promising for research community

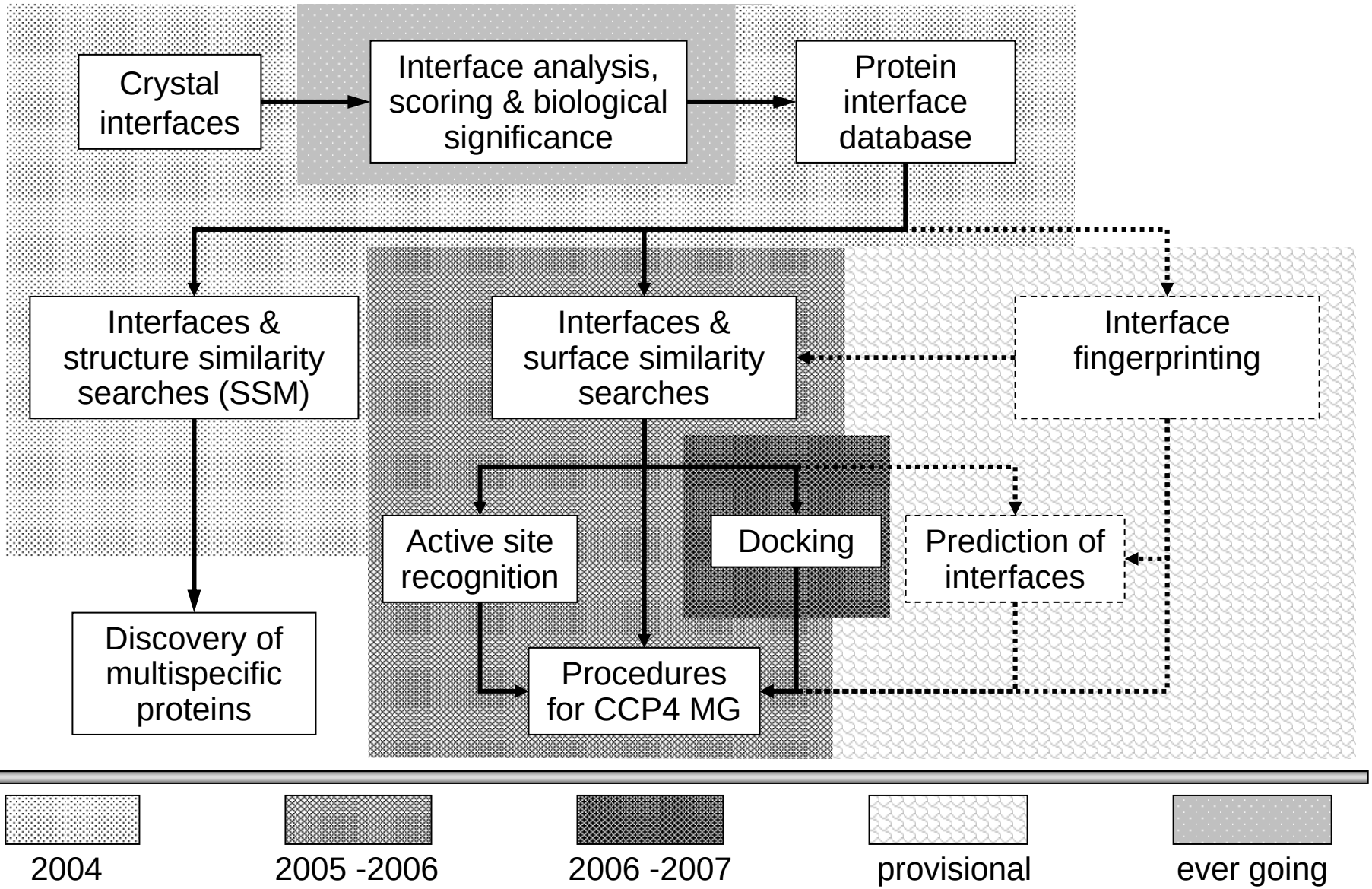
Collaboration at present with:

1. Laboratoire d'Enzymologie et Biochimie Structurales, Gif-sur-Yvette, France
2. Janet Thorton’s research group, EBI

Protein Interfaces: project scheme



Interactive Web server

provisional parts, subject to progress and feasibility

Protein Interfaces: project schedule