

MX data handling at SPring-8

Current status of Mail-in system and LIMS

Takashi Kumasaka
Structural Biology Group
SPring-8/JASRI

March 18th – 19th, 2008 APS/ANL

3WM 2008

Outline

1. Introduction

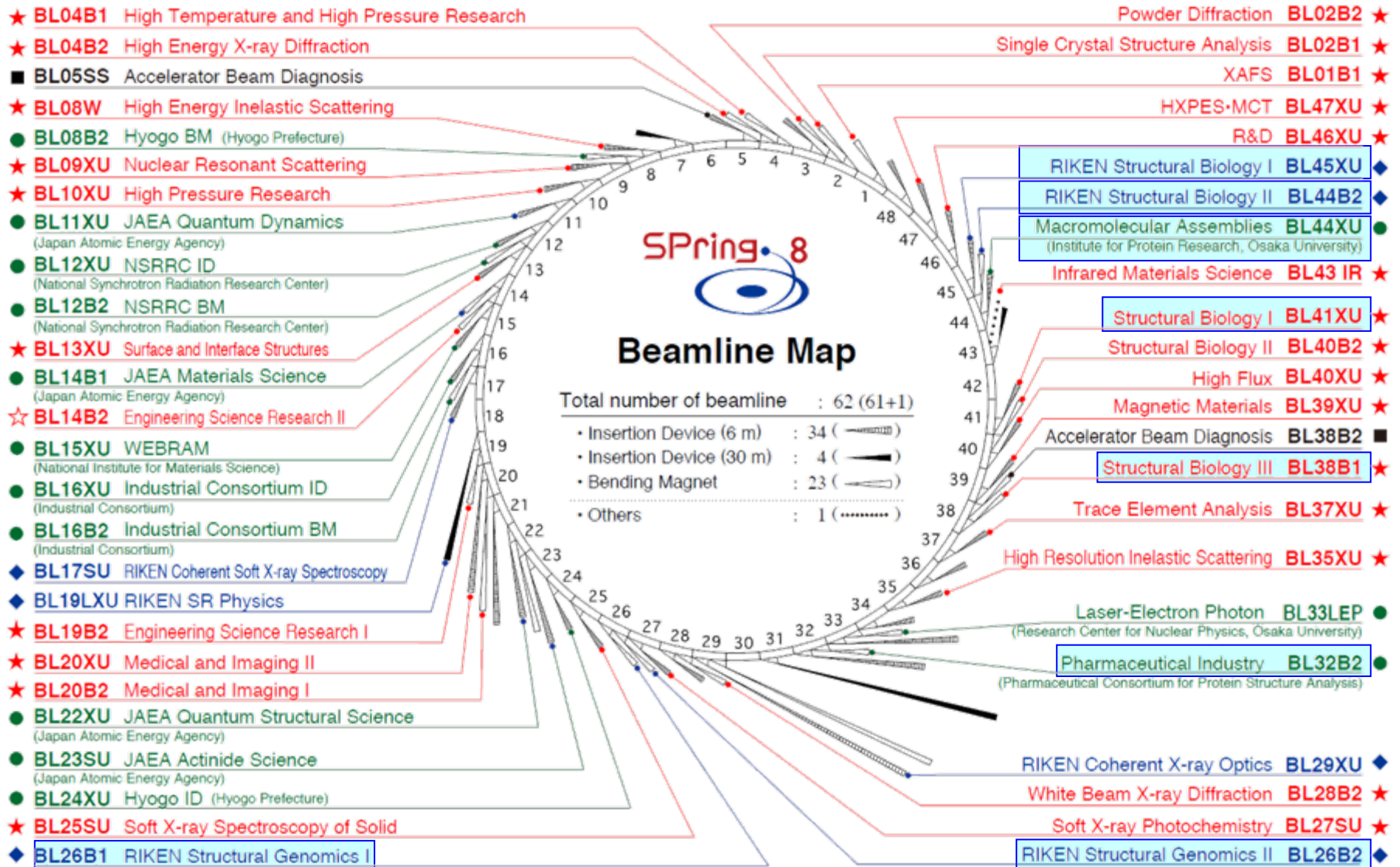
- i. PX BLs and their objectives

2. BL automation & LIMS

- i. BL automation
- ii. Mail-in system + BL LIMS

3. Summary and Future Plan

Beamlines at SPring-8



8 of 49 beamlines are fully dedicated to protein crystallography (as of March 2008)

Objectives of PX Beamlines at SPring-8

Undulator Beamlines

Objective: Advanced data collection on a case-by-case basis.

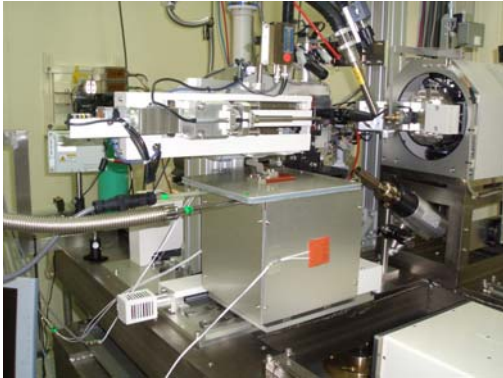
- Large unit cell crystals
- Micro crystals
- Ultra-high resolution structure analysis

Bending Magnet Beamlines

Objective: High-throughput & routine data collection

- Automated data collection & handling
- Remote BL operation

MX Automated Data Collection System



SPRING-8 MX beamline automation conducts with ...

Automated sample changer robot

Sample changer "SPACE"

(SPRING-8 Precise Automatic Cryo-sample Exchanger)

SPACE mounts, unmounts, and changes samples automatically

Integrated beamline control software

Beamline control software "BSS"

(Beamline Scheduling Software)

Job ID	Status	Mode	Crystal ID	Ther Position	From	To	Exp. Time	Wavelength
1	Success	Crystal Check	CO_0001	1	0.00	90.00	1.00	4.00
2	Success	XAFS	CO_0001	1	---	---	0.0001	1.0
3	Success	Crystal Check	CO_0002	2	0.00	90.00	1.00	4.00
4	Success	XAFS	CO_0002	2	---	---	0.0001	1.0
5	Success	Crystal Check	CO_0003	3	0.00	90.00	1.00	4.00
6	Success	Crystal Check	CO_0004	4	0.00	90.00	1.00	4.00
7	Success	Crystal Check	CO_0005	5	0.00	90.00	1.00	4.00
8	Success	Crystal Check	CO_0006	6	0.00	90.00	1.00	4.00
9	Success	Crystal Check	CO_0007	7	0.00	90.00	1.00	4.00
10	Waiting	Crystal Check	CO_0008	8	0.00	90.00	1.00	4.00
11	Waiting	Crystal Check	CO_0008	8	0.00	90.00	1.00	4.00
12	Waiting	XAFS	CO_0008	8	---	---	0.0001	1.0
13	Waiting	Crystal Check	CO_0009	9	0.00	90.00	1.00	4.00
14	Waiting	XAFS	CO_0009	9	---	---	0.0001	1.0
15	Waiting	Crystal Check	CO_0010	10	0.00	90.00	1.00	4.00
16	Waiting	XAFS	CO_0010	10	---	---	0.0001	1.0
17	Waiting	Crystal Check	CO_0011	11	0.00	90.00	1.00	4.00

Message Console

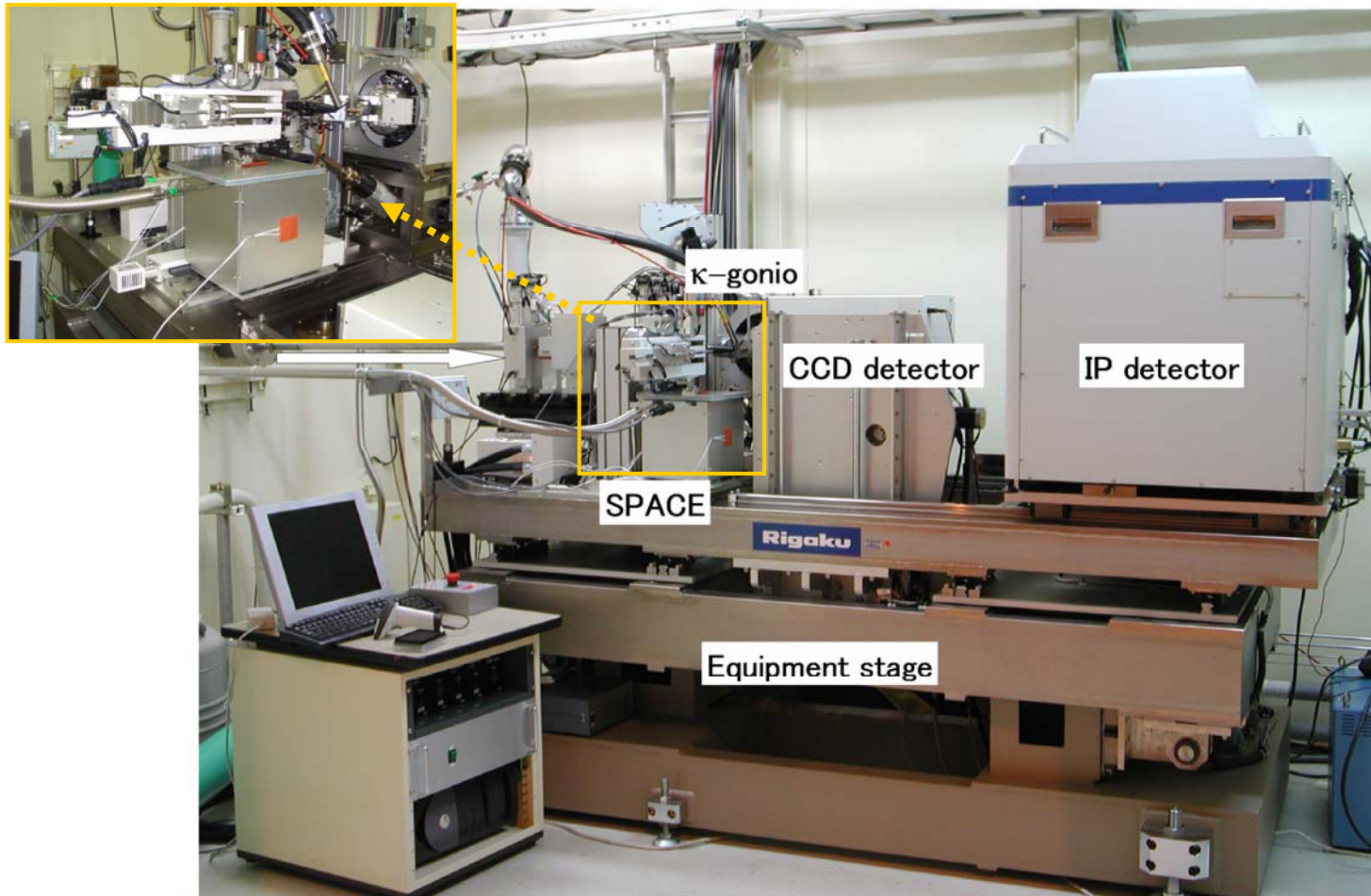
System Message | Job Message | Error Message

Set wavelength to 0.922841 [Job: 2004/09/10 P#4] 18:21:33
 Warning: Light is on. Forced to resume 2004/09/10 P#4 18:21:33
 Set wavelength to 0.922141 [Job: 2004/09/10 P#4] 18:21:33

Beamline components are controlled by BSS

Experimental Hutch (BL26B2)

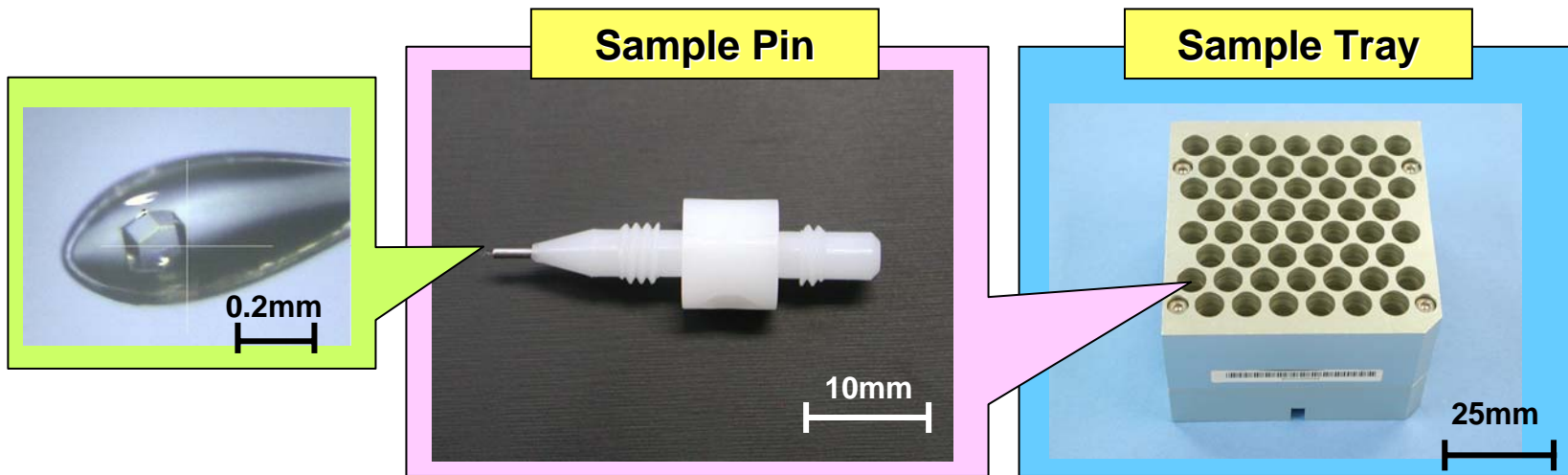
This beamline is suitable for rapid measurement



Overview of experimental stage equipped with SPACE

Automatic Sample Changer SPACE

SPACE = SPring-8 Precise Automatic Cryo-sample Exchanger
Automatic sample change with using high reproducibility of mounted crystal position (error: ~10 μ m)



Sample pin

- length 25mm
- diameter 7mm
- material polyoxymethylene (polyacetal)

Sample tray

- size 75 x 75 x 50 mm³
- weight 500g
- material aluminum
- 51 samples can be mounted + one for position adjustment

SPACE

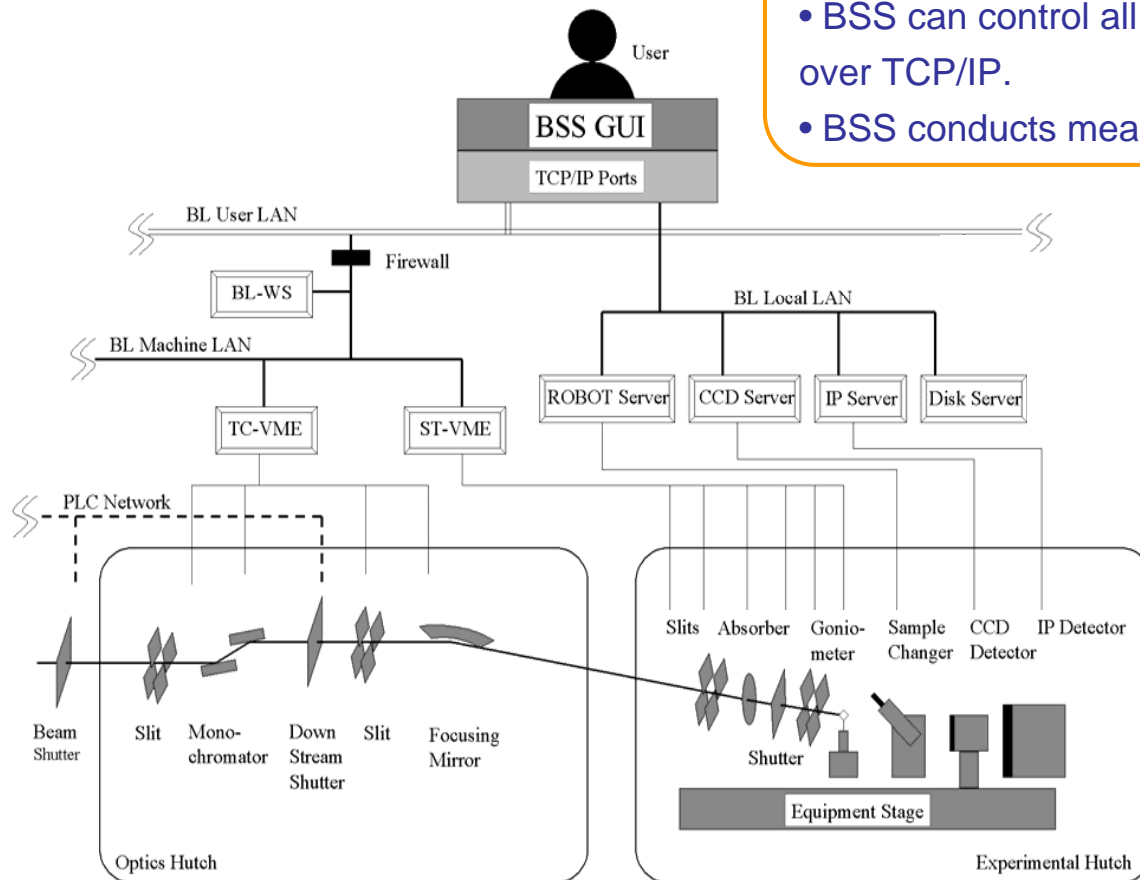
- Three axis robot and XY stage for sample storage.
- Up to two trays (102 samples) can be stored.
- Automatic liquid N₂ supply



Integrated Beamline Control Software BSS

BSS = Beamline Scheduling Software

- Client application with GUI
- User friendly interface
- BSS can control all components of beamline over TCP/IP.
- BSS conducts measurements on schedule.



Measurement Scheduling & Logging by BSS

User plans the order of measurements on these windows.

Conducting in descending order

Job ID	Status	Mode	Crystal ID	Tray Position	From	To	step	Exp. Time	Wavelength
1	Success	Crystal Check	CID_0001	1	0.00	90.00	1.00	4.00	1.00000
2	Success	XAFS	CID_0001	1	---	---	0.0001	1.0	0.97474 ---> 0.98474
3	Success	Crystal Check	CID_0002	2	0.00	90.00	1.00	4.00	1.00000
4	Success	XAFS	CID_0002	2	---	---	0.0001	1.0	1.27840 ---> 1.28840
5	Success	Crystal Check	CID_0003	3	0.00	90.00	1.00	4.00	1.00000
6	Success	Crystal Check	CID_0004	4	0.00	90.00	1.00	4.00	1.00000
7	Success	Crystal Check	CID_0005	5	0.00	90.00	1.00	4.00	1.00000
8	Success	Crystal Check	CID_0006	6	0.00	90.00	1.00	4.00	1.00000
9	Success	Crystal Check	CID_0007	7	0.00	90.00	1.00	4.00	1.00000
10	Waiting	XAFS	CID_0007	7	---	---	0.0001	1.0	0.97474 ---> 0.98474
11	Waiting	Crystal Check	CID_0008	8	0.00	90.00	1.00	4.00	1.00000
12	Waiting	XAFS	CID_0008	8	---	---	0.0001	1.0	0.97474 ---> 0.98474
13	Waiting	Crystal Check	CID_0009	9	0.00	90.00	1.00	4.00	1.00000
14	Waiting	XAFS	CID_0009	9	---	---	0.0001	1.0	0.97474 ---> 0.98474
15	Waiting	Crystal Check	CID_0010	10	0.00	90.00	1.00	4.00	1.00000
16	Waiting	XAFS	CID_0010	10	---	---	0.0001	1.0	0.97474 ---> 0.98474
17	Waiting	Crystal Check	CID_0011	11	0.00	90.00	1.00	4.00	1.00000

Current measurement

Measurement schedule

Modify

MODE: Manual, OPTION: Simulation, STATUS: Crystal Evaluation

Main window of BSS

Edit Schedule

Job ID# 4

Tray Position Not Used

Crystal ID# 1001001

Sample Name ip_single

Data Directory /image/

Mode Collection Detector Gonio XAFS HTPF

Scan from 0.0 to 5.0 step 1.0 [deg]

Camera distance 150.0 [mm]

Sampling interval 1 [points]

Wavelength [A]

#1: 1.00000 #2: 1.02000 #3: 1.04000 #4: 1.06000

Exposure time [sec]

#1: 4.0 #2: 4.0 #3: 4.0 #4: 4.0

Number of Wavelength 1

MAD interval 10 [points]

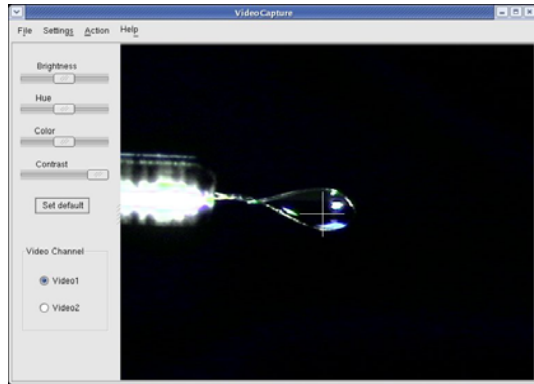
CCD 2 theta 0.0 [deg]

Apply Close Show List

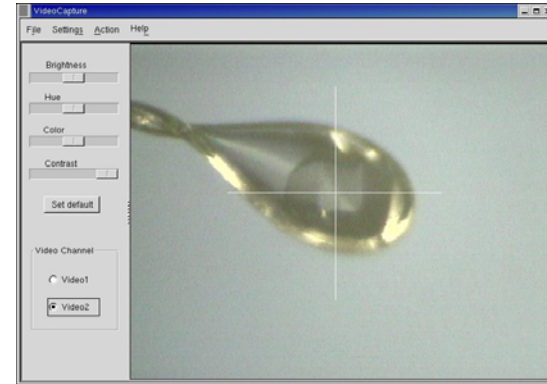
Schedule edit window

1. BSS conducts measurements on schedule.
2. Crystals are automatically changed by SPACE on BSS control.
3. Each measurement condition/result is output as a text file.

Screenshots of BSS

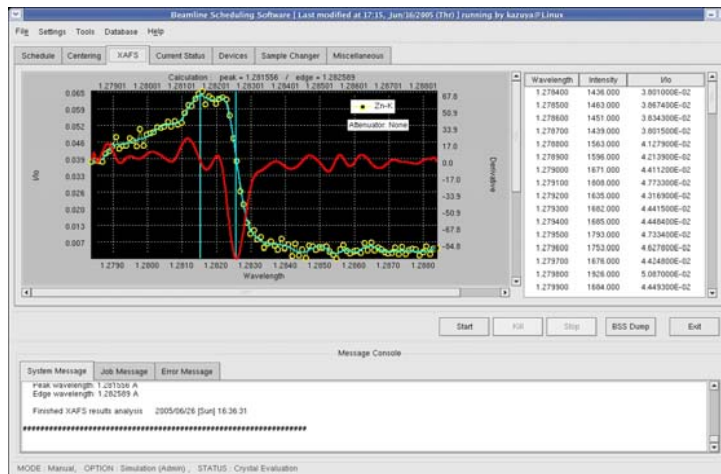


Low magnification microscope (Field of view 5 x 4 mm²)
Automatic loop centering

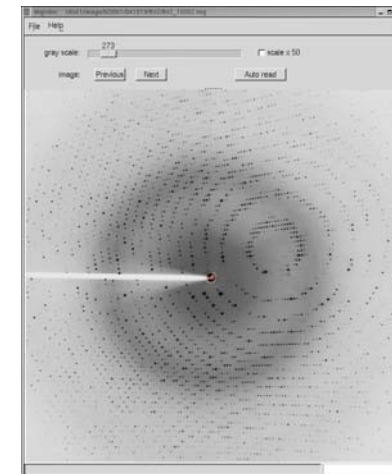


High magnification microscope (Field of view 0.6 x 0.5 mm²)
Click-on centering

Video monitoring and crystal-centering software



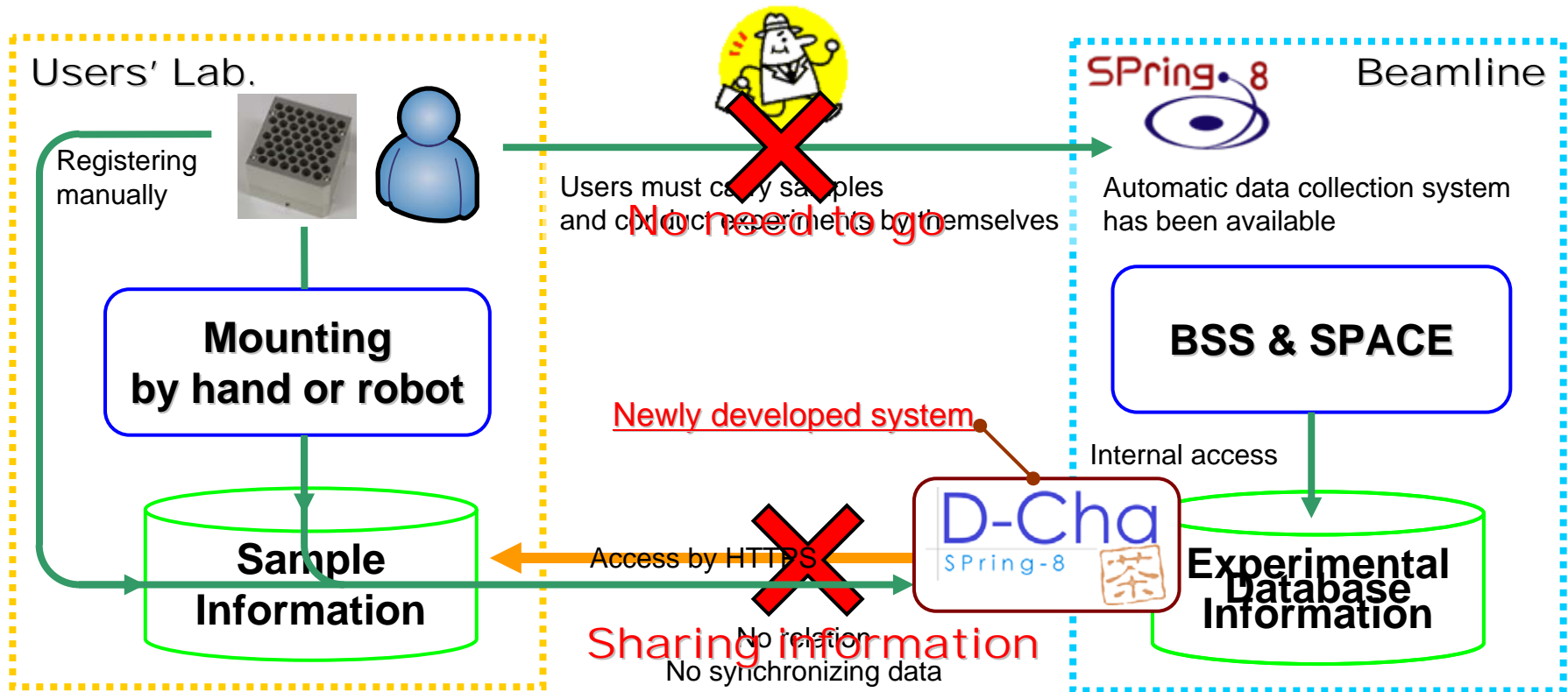
Measurement of XAFS spectrum



Diffraction image viewer + analysis

Mail-in Data Collection as a first step to remote bl operation

Present situation



Users can obtain the collected data with media or via the Internet.

Development of Interface & Concept of Mail-in Data Collection

The interface should be ...

- Can access sample information
- Can be used at home lab

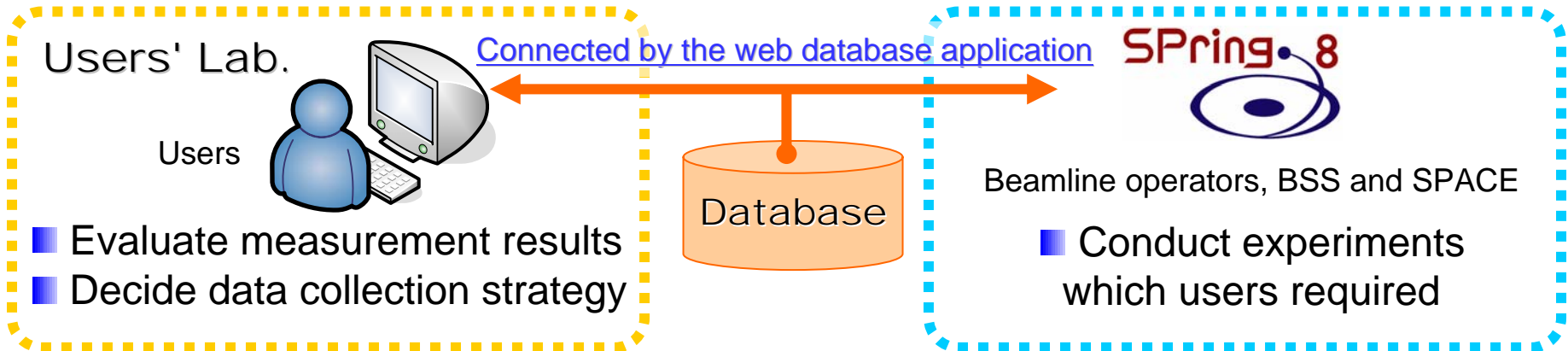


Has relational database
Works on the Internet



Web database application

SPring-8 mail-in overview with the web database application

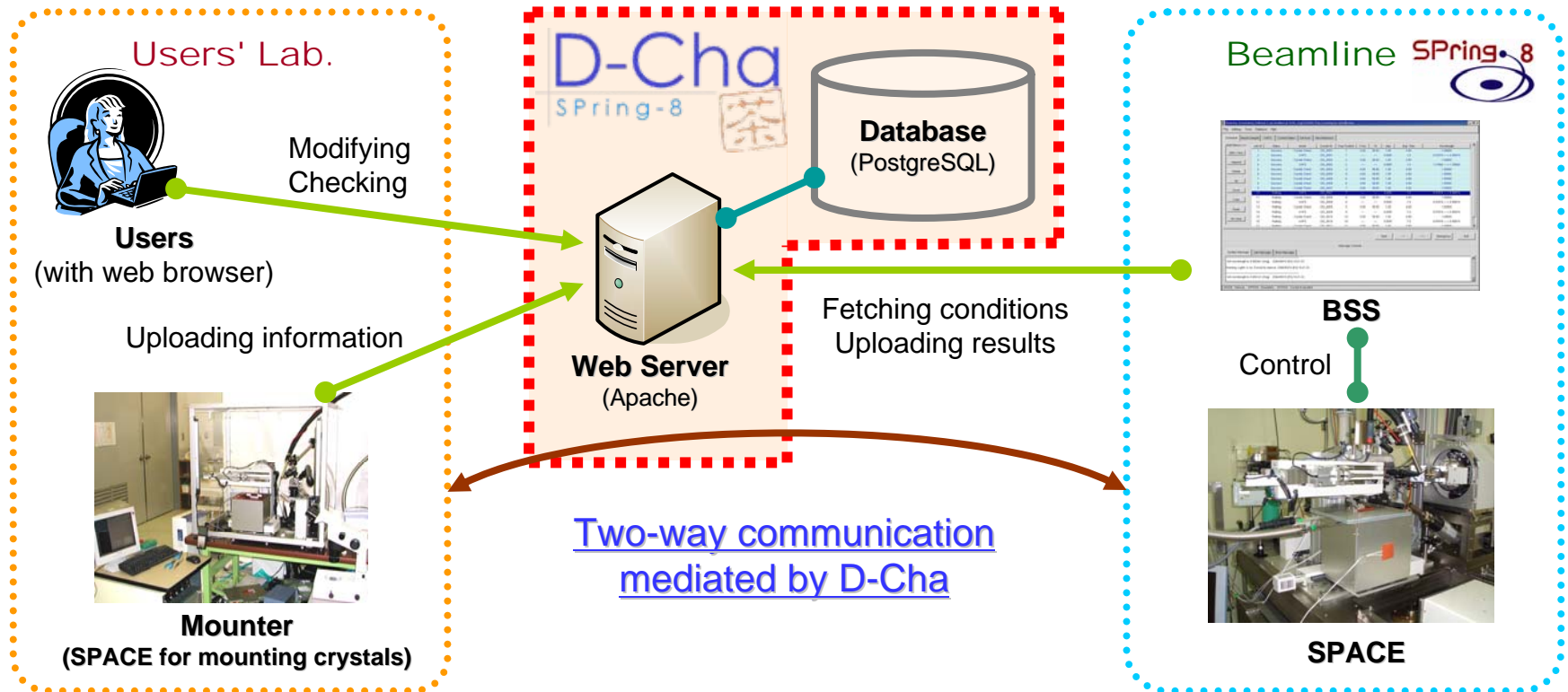


Our Concept: Remote operation with beamline operator's assist.

Development of Web Database

Database for Cystallography with Home-lab Arrangements

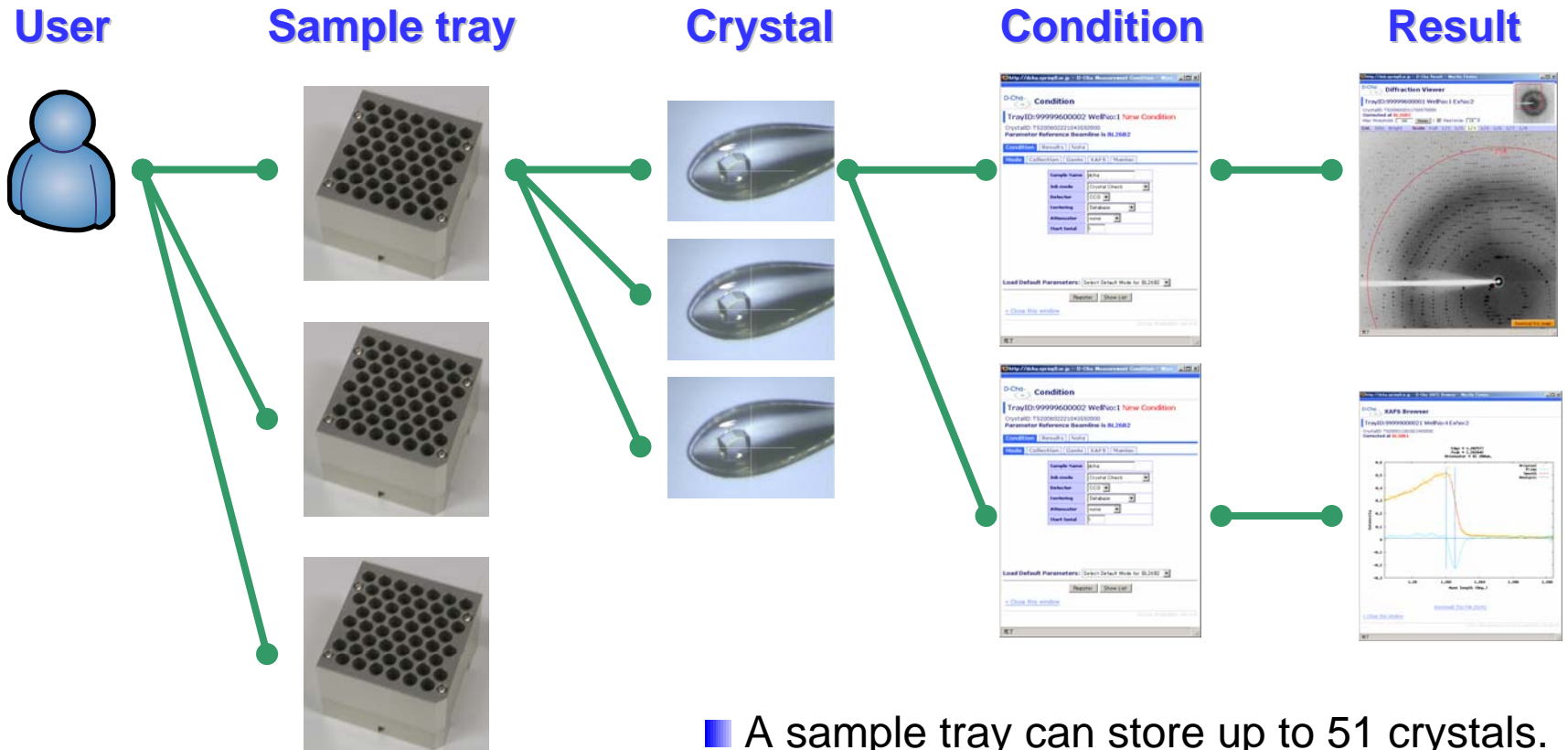
written in Perl on Linux and using some open source software



BSS and Mounter communicate with D-Cha in XML (like XML-RPC architecture).

What D-Cha Manages as a BL LIMS

D-Cha have to manage many sample information, measurement conditions as a BL LIMS (Laboratory Information Management System). It manages information in following structure.



- A sample tray can store up to 51 crystals.
- A crystal has some conditions.
- A conditions has the result.

D-Cha Screenshots (1)

D-Cha web interfaces

User Menu (Modify Trays, Crystals and Conditions)

D-Cha needs authentication

Login

Open tray manager

User Home

Users can browse and modify information for trays and crystals through D-Cha interface.

Registered tray list

Open crystal manager

TrayID	Comment	BL	GroupID	Check-in	Deadline (Check)	Deadline (Dataset)	Check-out
99999000020	TEST	BL26B2	99999				
99999000021		BL38B1	99999				
99999500002	Test Tray	Default	99999				
99999600002	BL26Test	BL26B2	99999				
99999600003		BL26B2	99999				

Registered tray list

Open crystal manager

D-Cha Screenshots (2)

Managing information and Setting condition

Tray ID: 99999600002

Crystals | Crystal Check | Dataset Collection | All Conditions | XAFS

TrayID	Well	CrystalID	CrystalShape	Protein	Resolution	Heavy Atom	Date	GroupID	UserID	Plan	Add Condition
99999600002	1	MovingTest					2006-02-22	99999	bluser	XA DC DS	-- Type --
99999600002	2	Test2					2006-02-22	99999	nobrin	DC M	-- Type --

DCha::CrystalManager ver.0.3

D-Cha ver.2.97.1 maintained by Nob-rin,2005-2006

Modifying Crystal Information



SPRING-8 Status

Tray ID: 99999600002

Crystals | Crystal Check | Dataset Collection | All Conditions | XAFS

No	CrystalID	Protein	Resolution	Heavy Atom	Well	ExNo	Condition	Status	Start	Finish	Resolution
1	MovingTest				1	1	XA Se Wavelength:0.974740 to 0.984740 step 0.000100	Success	06-02-22 11:11	06-02-22 11:17	
2	MovingTest				1	2	DC Jupiter210 Scan:0.00 to 90.00 w/1.00 s/90, 200.00mm, 1.000000Å, 4.0s	Success	06-02-22 11:18	06-02-22 11:20	
3	Test2				2	1	DC Jupiter210 Scan:0.00 to 90.00 w/1.00 s/90, 200.00mm, 1.000000Å, 4.0s	Success	06-02-22 11:20	06-02-22 11:25	

[UP] [DOWN] [Save Order]

D-Cha ver.2.97.1 maintained by Nob-rin,2005-2006

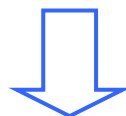
Progress and status

Modifying Measurement Conditions



Users can append/modify conditions.

Operator conducts measurements at SPRING-8...



Browsing results

3WM 2008

Users can modify measurement conditions through these web pages.

These pages are toggled by tab above the list. These pages summarize crystal information and conditions.

After measurement starting, users can browse the progress and status.

http://dcha.spring8.or.jp - D-Cha Measurement Condition - Mozilla

D-Cha Condition

TrayID:99999600002 WellNo:1 New Condition

CrystalID: TS200602221043550000

Parameter Reference Beamline is BL26B2

Condition | Results | Note

Mode | Collection | Goni | XAFS | Maniac

Sample Name: dcha

Job mode: Crystal Check

Detector: CCD

Centering: Database

Attenuator: none

Start Serial: 1

Load Default Parameters: Select Default Mode for BL26B2

Register Show List

> Close this window

DCha::ExpEditor ver.0.3

D-Cha Screenshots (3)

Users can browse results on these windows.

D-Cha Condition

TrayID:90002000001 WellNo:14 ExNo:1
 CrystalID:TS200511221142440000
 Parameter Reference Beamline is BL26B2

Set No	Wave	ExTime	Start	Osc.	Time Stamp	File
1	1	1.00000	4.0	-90.0	1.0	2005/11/24 14:22:48
1	2	1.00000	4.0	0.0	1.0	2005/11/24 14:23:14

File	Size	Time Stamp	Type
sample_image_000.ppm	864121	2005-11-24 14:16:31	Snapshot
sample_image_000_back.ppm	864015	2005-11-24 14:16:33	Snapshot

Close this window

DCha:ExpEditor ver.0.3

Simple File Manager



Browse

D-Cha Diffraction Viewer

TrayID:99999600001 WellNo:1 ExNo:2
 CrystalID:TS200602011720570000
 Corrected at BL26B2

Max threshold: 040 Check ResCircle: 25 Å

Cnt. Dim Bright Scale Full 1/2 1/3 1/4 1/5 1/6 1/7 1/8

2.5 Å

Diffraction Viewer

Can change contrast, magnify, draw resolution circle
 Scrolling with dragging mouse

Contrast, Scale, Resolution Circle Parameters

Overview Image

D-Cha XAFS Browser

TrayID:99999000021 WellNo:4 ExNo:2
 CrystalID:TS200511301621420000
 Corrected at BL30B1

Edge = 1.282577
 Peak = 1.282042
 Attenuator = Al 200um.

Intensity

Wave Length (Å)

Original
 Fit Line
 Smooth

Download This File (RAW)

Close this window

XAFS Browser

Can show wavelength with click

D-Cha File Browser

TrayID:99991000001 WellNo:2 ExNo:1
 CrystalID:DEMOCCDIMAGE0000000002
 Corrected at BL26B2

Download This File (RAW)

Close this window

DCha:FileBrowser ver.0.3-PkafPLOT

Crystal Snapshot

Users can download raw data through these pages.

A performance of Mail-in system

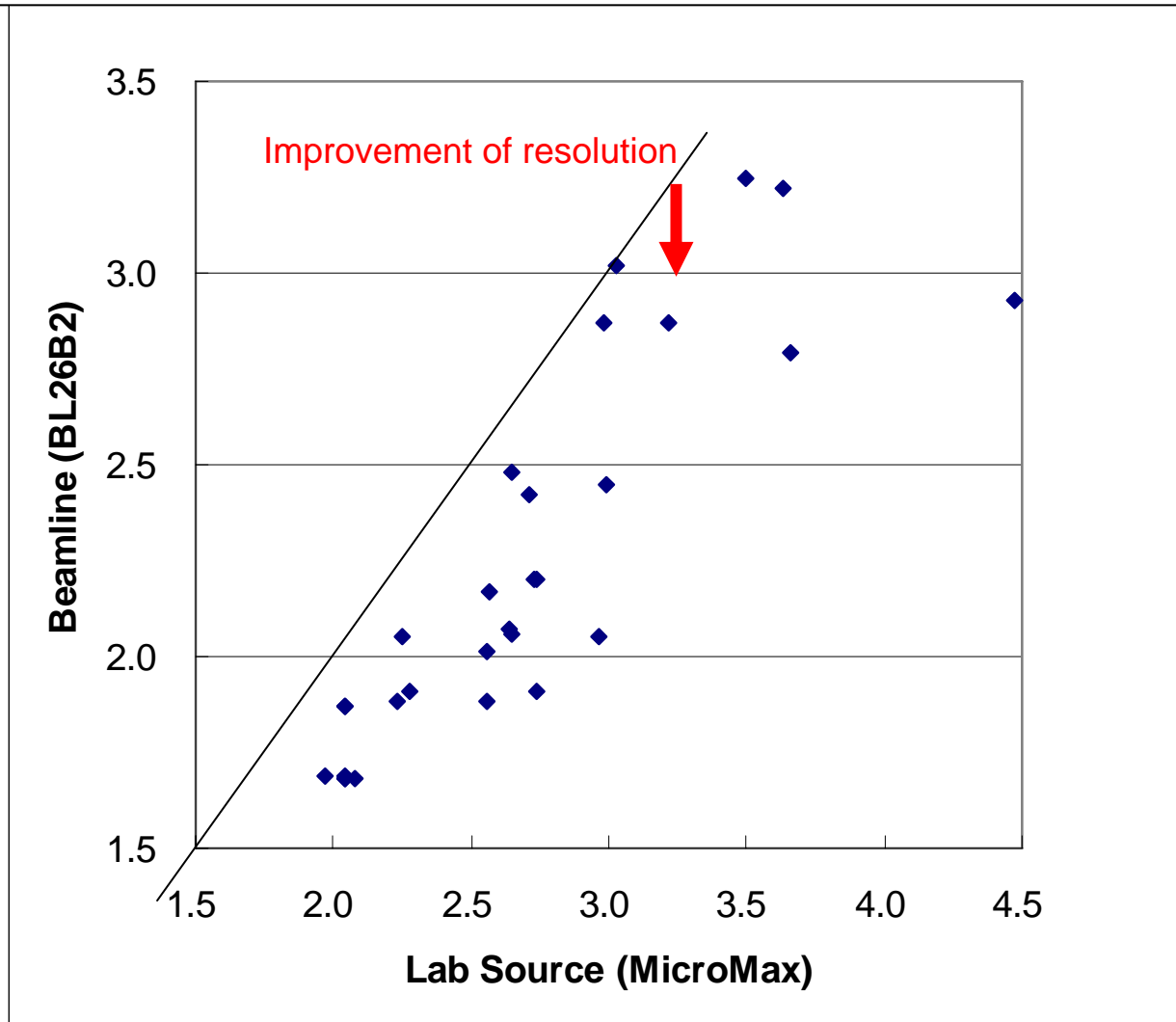
A structural biology group performs MX data collection in a week:

No. of checked samples/types	205/13
No. of data sets collected at BL	22
Ratio of No. data/samples	11%

A effective crystal selection scheme should be required.

A preliminary result of data mining

Relationship of crystal resolution using a beamline and lab X-ray.



Summary and Future Plan

Summary

- D-Cha is a web database to connect distant users to beamline.
- BSS, SPACE and D-Cha made it possible to collect data without visiting SPring-8.
- D-Cha works as BL LIMS also.

Future Plan

- Integration with a diffraction image analysis software.
- Development of expert system integrated with BL LIMS.
- Development of a complete remote access system based on D-Cha.

Staff

SPring-8/RIKEN

Go Ueno

Hironori Murakami

Takaaki Hikima

Masaki Yamamoto

SPring-8/JASRI

Kazuya Hasegawa

Seiki Baba

Nobuo Okazaki (former member)

Takashi Kumasaka

PharmAxess Inc (BL operation)

Raita Hirose

Yuki Nakamura