

# Data acquisition/analysis software for Diffraction Beam Lines at SSRL

**Certified**  
*Scientific Software*

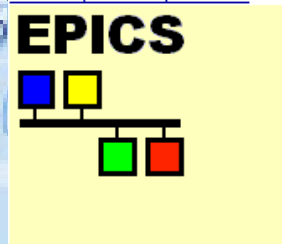


**SPECPLOT**

**spec**

**ICS**

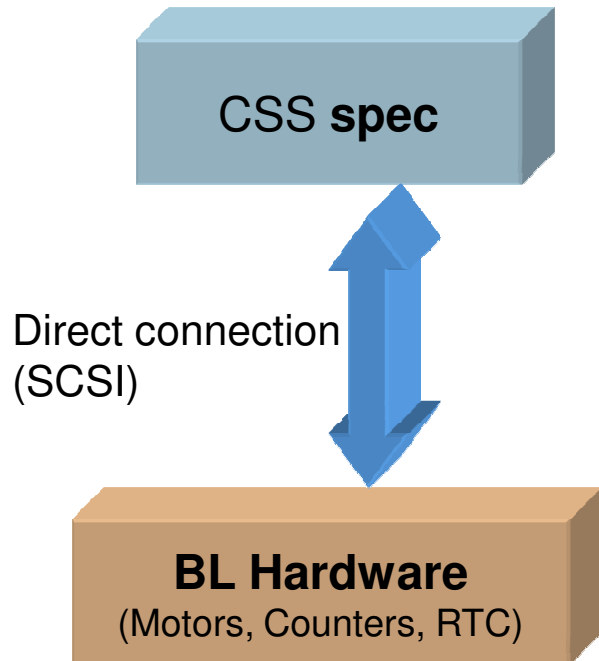
**WebSpec**



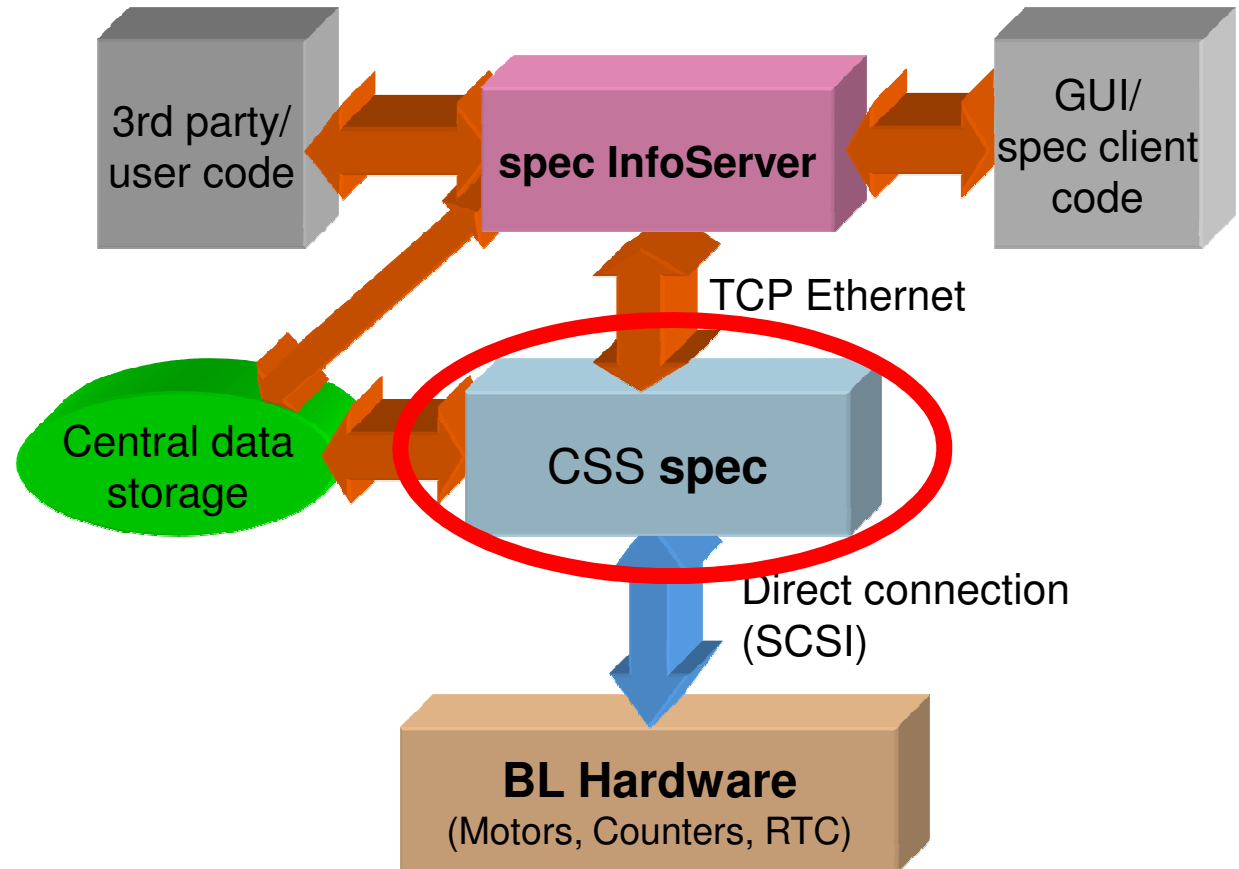
**WxDiff**

# Beam line control scheme with spec

First installation on BL 2-1



Current layout on spec diffraction beamlines



spec

<http://www.certif.com>



- \* Commercial program from Certified Scientific Software.
- \* Instrument control package to move motors, use all kind of detectors (counters, MCA, CCD)
- \* Routines to scan these devices, plot, save the data, work with diffractometers in reciprocal space (n-circle, kappa, z-axis,) etc.
- \* Command Line Interface
- \* Powerful macro language to automate data taking, powerful data handling routines to analyze data on line. Generic serial and ethernet communication routines.
- \* More recently: server-mode; allows control over spec from remote machine!
- \* **Important SSRL additions:** automatic absorbers, calibration macros, creation of .csv files (Excel), motor monitor, access to third party software via multi-client server interface.

# spec

**Motor monitor**

tth	th	table	gonx	gony	gonchi	gonthe	zstage	m0vsl	m0hsl
0.0000	90.0000	0.5837	0.0001	-0.6220	0.0000	0.0000	10.0000	-0.4826	1.5000
l0h	r0h	t0v	b0v	h0gap	h0tran	v0gap	v0tran	l1h	r1h
2.0000	2.0000	1.7500	1.7500	4.0000	0.0000	3.5000	0.0000	5.0000	5.0000
t1v	b1v	h1gap	h1tran	v1gap	v1tran	l2h	r2h	t2v	b2v
2.0000	2.0000	10.0000	0.0000	4.0000	0.0000	5.0000	5.0000	2.0000	2.0000
h2gap	h2tran	v2gap	v2tran	_0	crystal	mono	SPEAR		
10.0000	0.0000	4.0000	0.0000	0.0000	14.3078	8000.0010	0.0128		

**Terminal**

```
Welcome to "spec" Release 5.08.04-4
Copyright (c) 1987-2009 Certified Scientific Software
All rights reserved

(Portions derived from a program developed at Harvard University.)
(Linked with BSD libedit library for command line editing.)

Using "/usr/local/lib/spec.d" for auxiliary file directory (SPECED).

Getting configuration parameters from "SPECED/twoc/config".
Can't open serial device "/dev/tty50". Permission denied.
Using Galil MC2280sG7b at "192.168.1.19".
Using JORWAY 73A Rev 300.
Warning: Timer "sec" not associated with master timer.
Warning: Monitor "mon" not associated with master timer.

Using two-circle configuration.

=
spec Hot Line: (617) 576-1610.
Type h changes for info on latest changes.
Browse to http://www.certif.com for complete documentation.
=

Reading file "SPECED/site.mac".
This is SSRL's BL2-1 site macro V0.064
User: SSRL\checkout, Time: Tue Jun 01 17:50:53 2010

Shared memory ID for motor      : 26345486
Shared memory ID for m. status  : 26378253
Shared memory ID for counters   : 26411020

1332.TWOC> ascan tth 0 5 20 1
Total 21 points, 21 seconds

Scan 1 Tue Jun 01 17:51:11 2010 file = checkout_060110 twoc user = SSRL\checkout
ascan tth 0 5 20 1

# TwoTheta Detector Monitor Seconds Fluor-De I2 Foils Normaliz Temp1
Been waiting 15 seconds for beam ...
```

**Command line interface**

# The most important **spec** commands

All movements and countings can be aborted by typing CTRL-C / STRG-C

**mv** *motor dest*

Moves motor *motor* to the absolute *dest* (umv update move).

**mvr** *motor delta*

Moves motor *motor* relative to current position. (umv update move relative).

**wm** *motor [motor2 motor3 . . .]*

Prints user and dial position of one or several motors (where motor)

**wa**

Prints user and dial position of all motors (where all).

**set** *motor value*

Sets the current user coordinates position of *motor* to *value*

**ct** [*time*]

Start counting on all counters for *time* seconds. (count)

**ascan** *motor start finish interv time*

Scans in absolute coordinates.

**dscan** *motor start finish interv time*

Scans relative to current position.

**newfile** *filename*

Sets a new data file

**plotselect** [*detector . . .*]

Selects detector(s) to be plotted.

**pplot** [*scan nr*]

Print plot

# spec scripting facility

## 1. Put file tempscan.mac in your home folder

```
def set_temp(setpt) '{
  # here goes some hardware-specific code for your temperature controller
  ser_par(0, "flush") # remove left-over characters
  sleep(0.05) # sleep to make sure that we do not initiate serial communication too often!
  ser_put(0, sprintf("SETP 1, %f\n",setpt)) # serial command to Lakeshore 340
}'

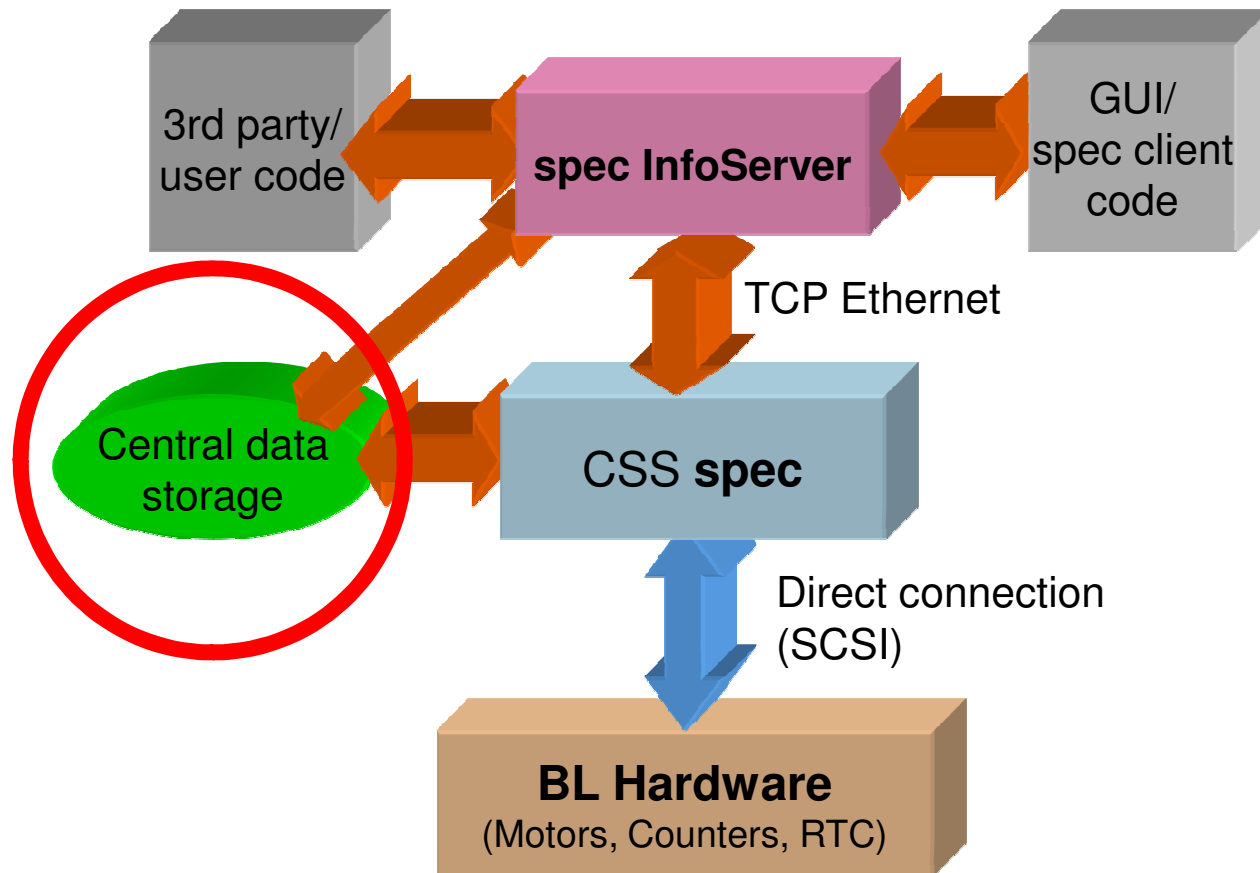
def temp_scan(fname, startT, endT, stepw) '
  if (!open(fname)) {
    p "Error opening file."
    return
  }
  for (currT = startT; currT <= endT; currT += stepw) {
    set_temp(currT)
    sleep(60) # wait for equilibration
    ct 2      # count for 2 seconds
    fprintf(fname, "%u\n", S[det])
  }
  close(fname)
'
```

## 2. Back in spec:

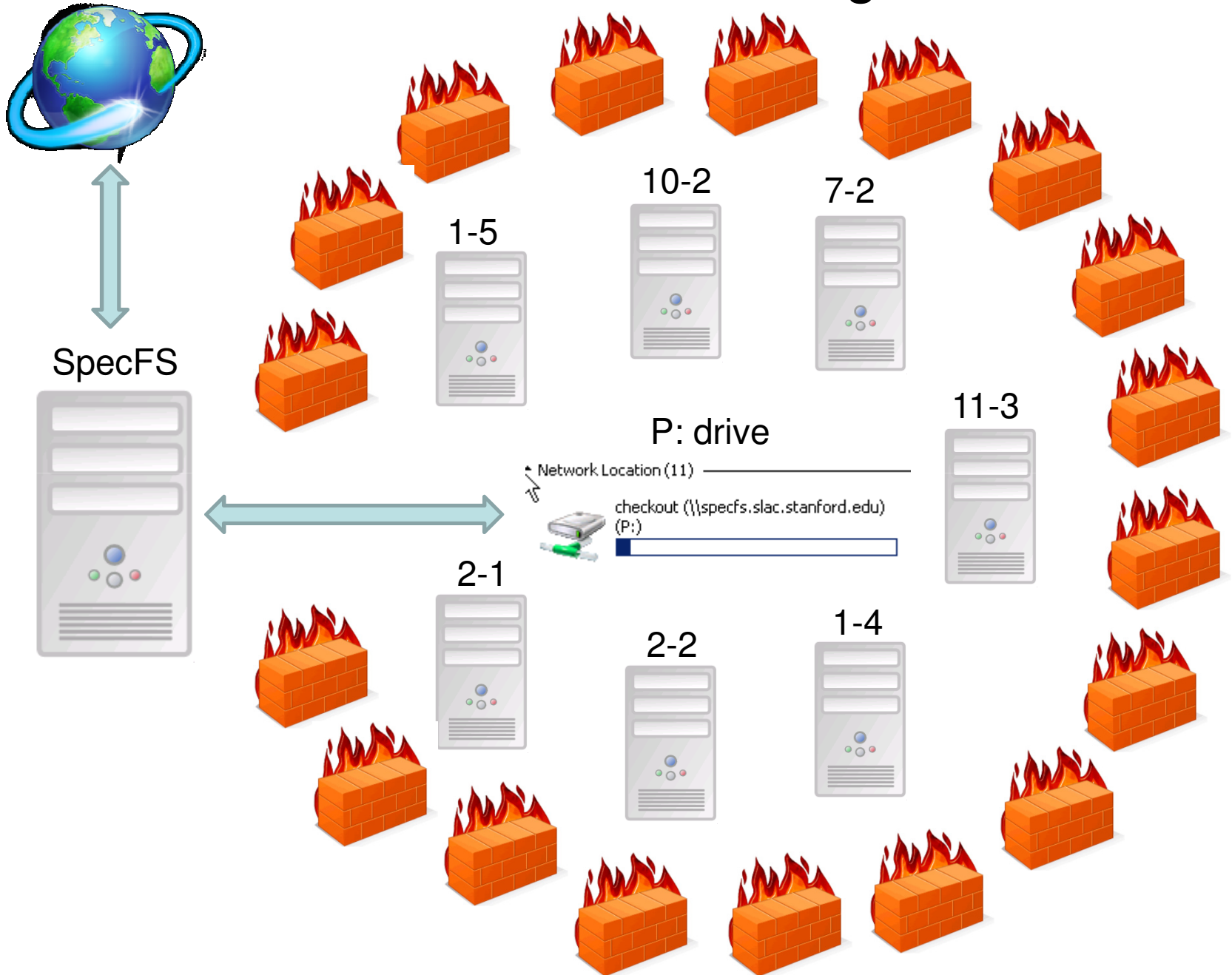
```
> dofile("~/tempscan.mac")
> temp_scan
```

# Beam line control scheme with spec

Current layout on spec diffraction beamlines



# Central data storage



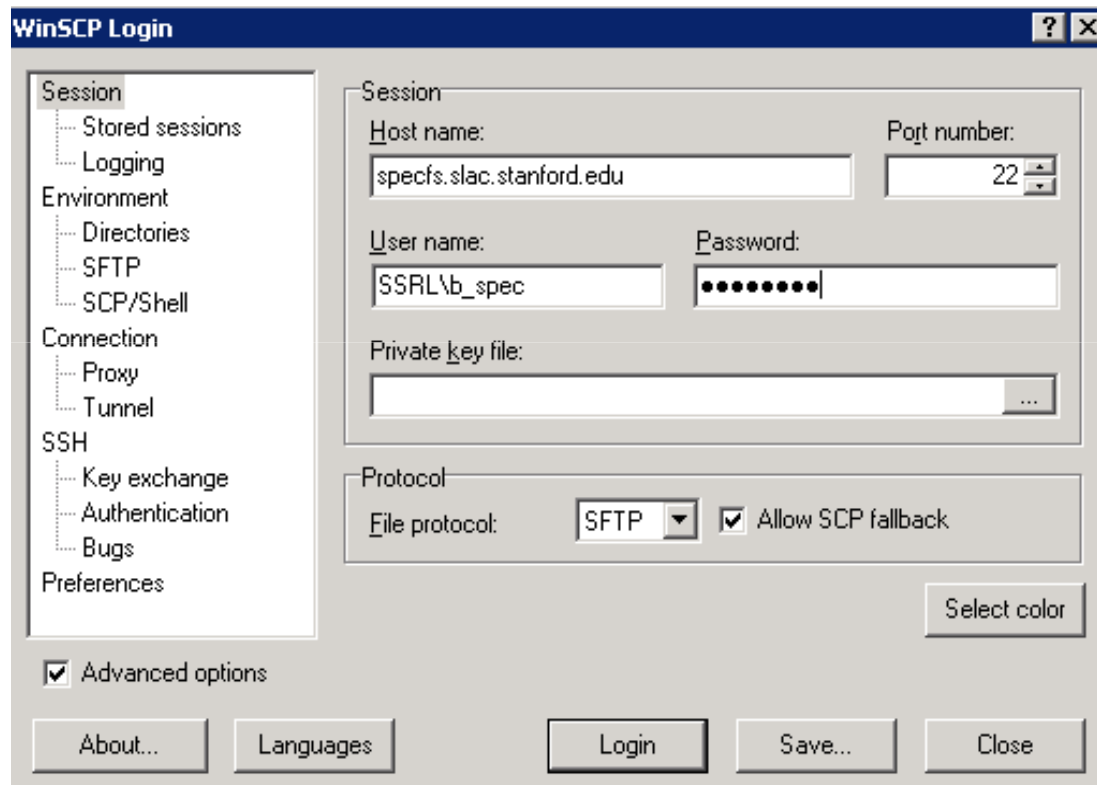


# Central data storage

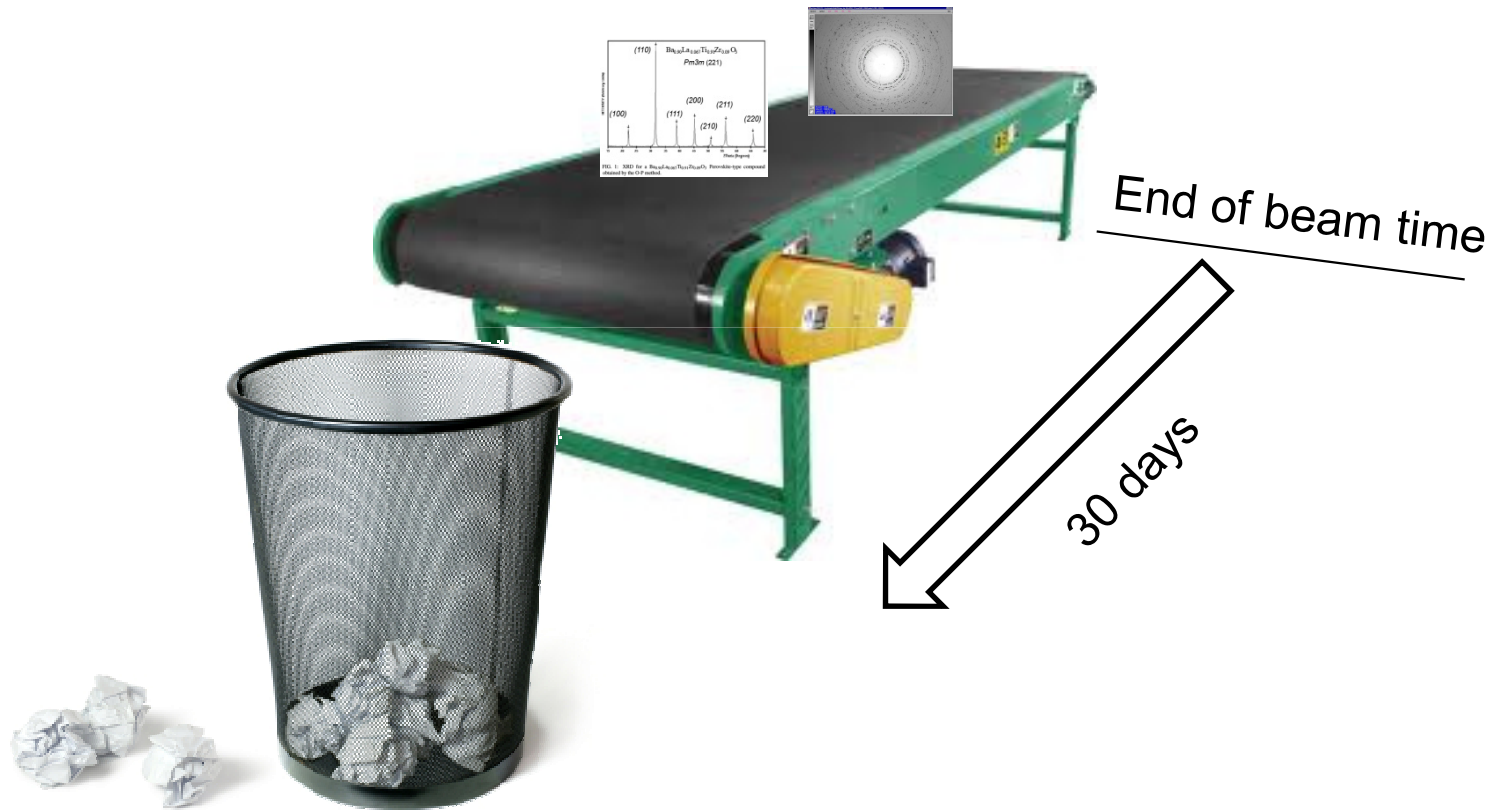
SFTP client, e.g. freeware WinSCP

<http://winscp.net/eng/download.php>

Start WinSCP, and enter

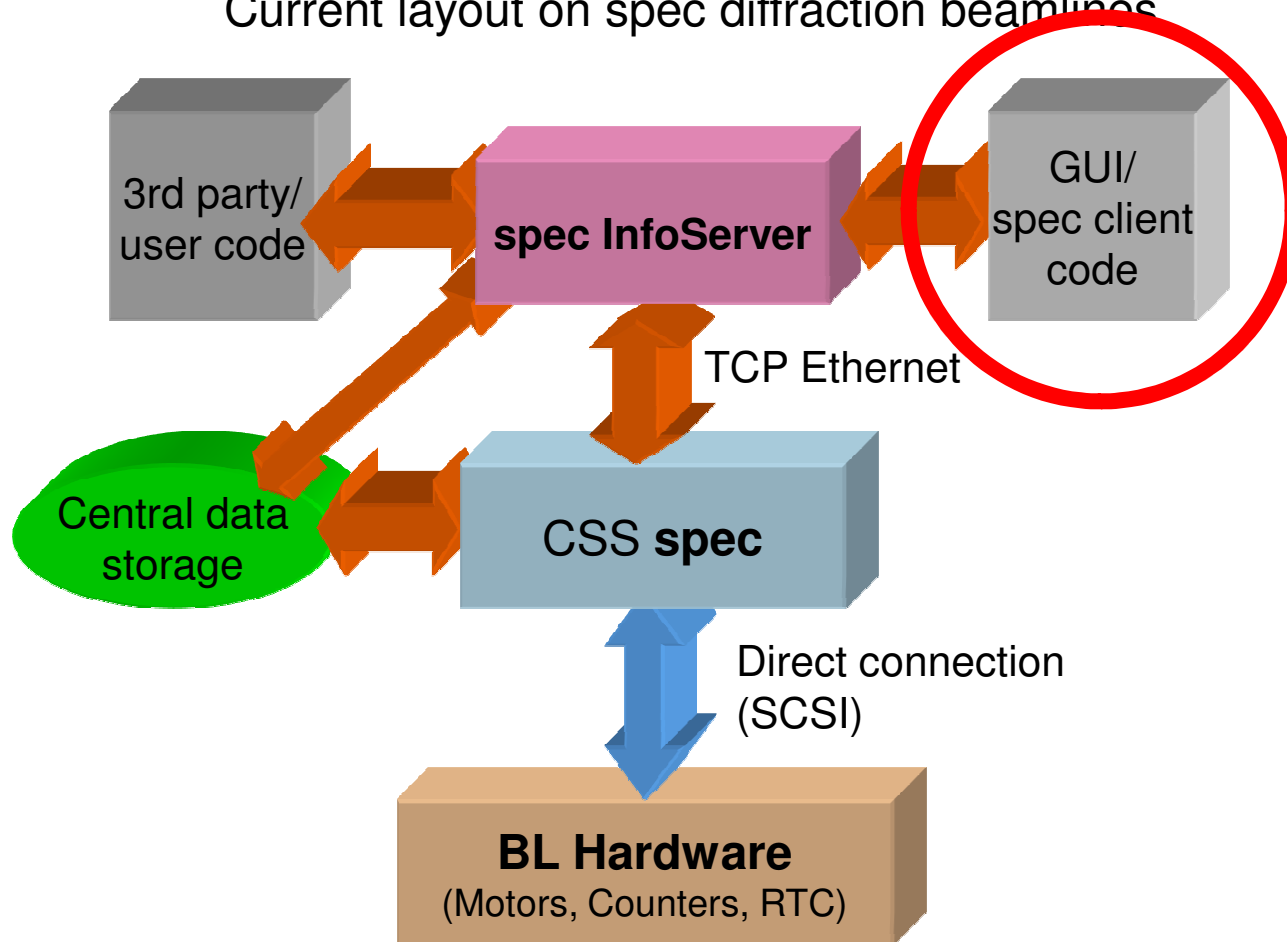


# Central data storage = temporary storage!



# Beam line control scheme with spec

Current layout on spec diffraction beamlines



# Data acquisition and visualization at BL 2-1, 2-2, 7-2, 10-2

2 PC setup: data collection and analysis on separate machines

**Linux** box running **spec** and supporting low-level Python code



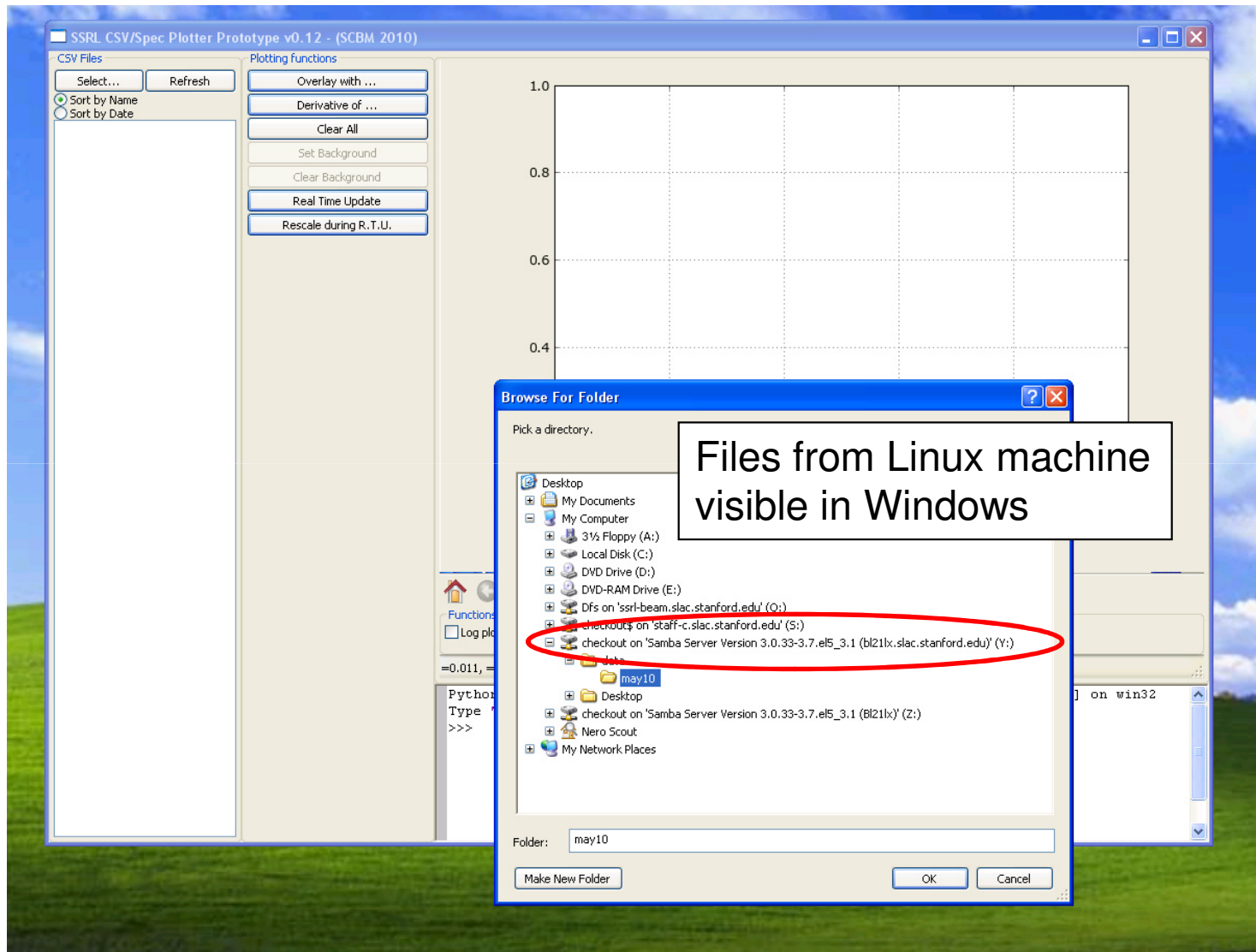
NFS, Samba



**Windows 7** box running **SpecPlot**



# SpecPlot

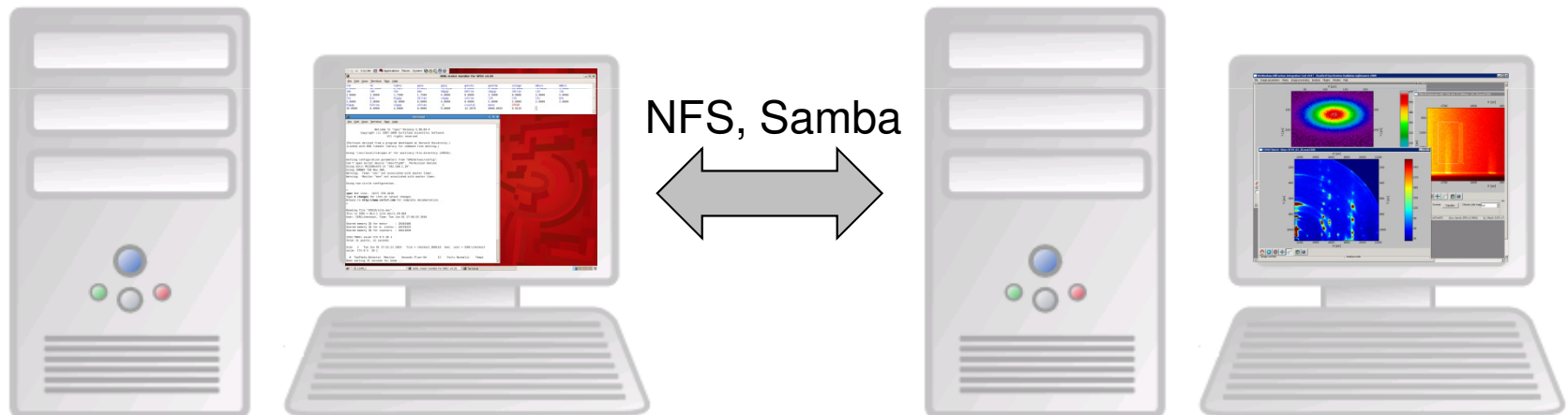


# Data acquisition and visualization at BLs 1-5, 11-3

New 2 PC setup: data collection and analysis on separate machines

**Linux** box running **spec** and supporting low-level Python code!

**Windows 7** box running **WxDiff** with Blue-Ice style GUI



## Appendix: Python Web Links



<http://www.pythonxy.com/>

All-in-one distribution for Windows, containing all the common scientific packages. Recommended!

<http://mathesaurus.sourceforge.net/matlab-numpy.html>

Useful list of MATLAB commands and their counterparts in the Python Module **NumPy** (part of the pythonxy package)

<http://zetcode.com/tutorials/pythontutorial/>

<http://zetcode.com/wxpython/>

Good collection of tutorials on the language and one of the available GUI packages, WxPython.