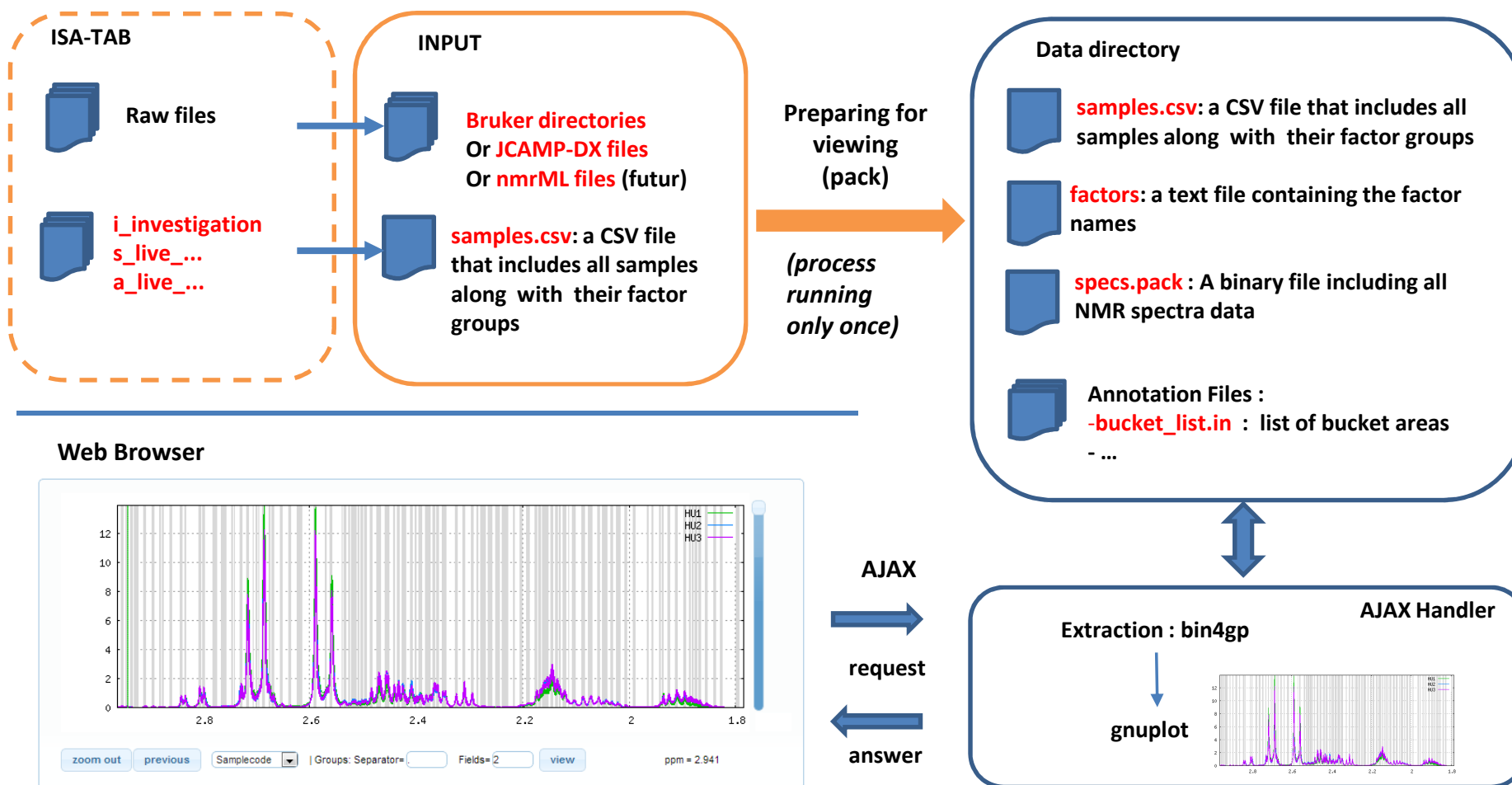


NMRViewer 1.0 - (C) INRA UMR 1332

Daniel Jacob

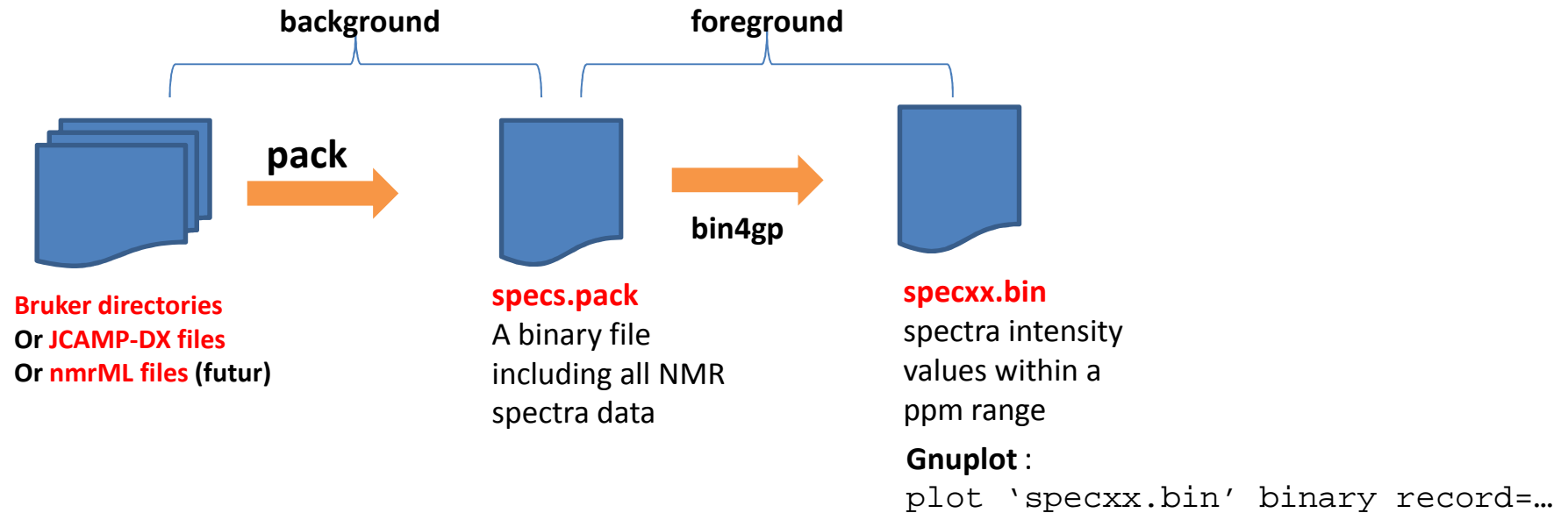
NMR spectra viewer : An overview of how it works



Web design based on the jQuery framework (client side) , PHP, C, gnuplot 4.3 (server side)

NMR spectra viewer : Why it runs so fast ?

➔ Because **Text to Binary conversion is time consuming**, so we do not manipulate data as text format but **only as binary format in foreground process**.
Text to Binary conversion is set up in a background process, only once.



➔ Trade off between consistency and efficiency

NMR spectra viewer : How to process with an ISA-TAB archive ?

Step 1: unzip the isatab archive

```
[djacob@proticdb nmrview]$ ll ./data/HUGO07/isatab/
total 11472
-rw-r--r-- 1 djacob users 317389 Mar 26 14:56 BB_BBI_08M07_melon07_13091.zip
-rw-r--r-- 1 djacob users 317361 Mar 26 14:56 BB_BBI_08M07_melon07_13092.zip
-rw-r--r-- 1 djacob users 318559 Mar 26 14:56 BB_BBI_08M07_melon07_13101.zip
-rw-r--r-- 1 djacob users 318787 Mar 26 14:56 BB_BBI_08M07_melon07_13102.zip
-rw-r--r-- 1 djacob users 318251 Mar 26 14:56 BB_BBI_08M07_melon07_13111.zip
-rw-r--r-- 1 djacob users 318122 Mar 26 14:56 BB_BBI_08M07_melon07_13112.zip
-rw-r--r-- 1 djacob users 309234 Mar 26 14:56 BB_BBI_08M07_melon07_13121.zip
-rw-r--r-- 1 djacob users 318059 Mar 26 14:56 BB_BBI_08M07_melon07_13122.zip
-rw-r--r-- 1 djacob users 318926 Mar 26 14:56 BB_BBI_08M07_melon07_13131.zip
-rw-r--r-- 1 djacob users 309249 Mar 26 14:56 BB_BBI_08M07_melon07_13132.zip
-rw-r--r-- 1 djacob users 317804 Mar 26 14:56 BB_BBI_08M07_melon07_13141.zip
-rw-r--r-- 1 djacob users 318394 Mar 26 14:56 BB_BBI_08M07_melon07_13142.zip
-rw-r--r-- 1 djacob users 323837 Mar 26 14:56 BB_BBI_08M07_melon07_13151.zip
-rw-r--r-- 1 djacob users 325276 Mar 26 14:56 BB_BBI_08M07_melon07_13152.zip
-rw-r--r-- 1 djacob users 324708 Mar 26 14:56 BB_BBI_08M07_melon07_13161.zip
-rw-r--r-- 1 djacob users 323442 Mar 26 14:56 BB_BBI_08M07_melon07_13162.zip
-rw-r--r-- 1 djacob users 324762 Mar 26 14:56 BB_BBI_08M07_melon07_13171.zip
-rw-r--r-- 1 djacob users 323527 Mar 26 14:56 BB_BBI_08M07_melon07_13172.zip
-rw-r--r-- 1 djacob users 324286 Mar 26 14:56 BB_BBI_08M07_melon07_13181.zip
-rw-r--r-- 1 djacob users 322688 Mar 26 14:56 BB_BBI_08M07_melon07_13182.zip
-rw-r--r-- 1 djacob users 323630 Mar 26 14:56 BB_BBI_08M07_melon07_13191.zip
-rw-r--r-- 1 djacob users 324020 Mar 26 14:56 BB_BBI_08M07_melon07_13192.zip
-rw-r--r-- 1 djacob users 324789 Mar 26 14:56 BB_BBI_08M07_melon07_13201.zip
-rw-r--r-- 1 djacob users 324475 Mar 26 14:56 BB_BBI_08M07_melon07_13202.zip
-rw-r--r-- 1 djacob users 311251 Mar 26 14:56 BB_BBI_08M07_melon07_13331.zip
-rw-r--r-- 1 djacob users 316116 Mar 26 14:56 BB_BBI_08M07_melon07_13332.zip
-rw-r--r-- 1 djacob users 311180 Mar 26 14:56 BB_BBI_08M07_melon07_13341.zip
-rw-r--r-- 1 djacob users 314663 Mar 26 14:56 BB_BBI_08M07_melon07_13342.zip
-rw-r--r-- 1 djacob users 319548 Mar 26 14:56 BB_BBI_08M07_melon07_13351.zip
-rw-r--r-- 1 djacob users 317141 Mar 26 14:56 BB_BBI_08M07_melon07_13352.zip
-rw-r--r-- 1 djacob users 326022 Mar 26 14:56 BB_BBI_08M07_melon07_13361.zip
-rw-r--r-- 1 djacob users 324277 Mar 26 14:56 BB_BBI_08M07_melon07_13362.zip
-rw-r--r-- 1 djacob users 320622 Mar 26 14:56 BB_BBI_08M07_melon07_13371.zip
-rw-r--r-- 1 djacob users 310643 Mar 26 14:56 BB_BBI_08M07_melon07_13372.zip
-rw-r--r-- 1 djacob users 319364 Mar 26 14:56 BB_BBI_08M07_melon07_13381.zip
-rw-r--r-- 1 djacob users 319049 Mar 26 14:56 BB_BBI_08M07_melon07_13382.zip
-rw-r--r-- 1 djacob users 8414 Mar 26 14:56 a_hugo_2007_metabolite_profiling_NMR_spectroscopy.txt
-rw-r--r-- 1 djacob users 10906 Mar 26 14:56 i_Investigation.txt
-rw-r--r-- 1 djacob users 5023 Mar 26 14:56 s_Hugo_2007.txt
```

Step 2: Preparing for viewing

```
[djacob@proticdb nmrview]$ sh ./scripts/buildcsv.sh -d ./data/HUG007/isatab/ -o samples.csv -v
i_Investigation.txt ... OK
s_Hugo_2007.txt ... OK
a_hugo_2007_metabolite profiling_NMR spectroscopy.txt ... OK
Extract columns from Study Assay File : 1,28 ...OK
Factors: ;Harvest date
Extract columns from Study File : 9,10 ... OK
Merging ...OK
```



```
[djacob@proticdb nmrview]$ sh ./scripts/init_bin.sh -i ./data/HUG007/isatab/samples.csv -o ./data/HUG007/procs/ -h
```

```
-----
BB_BBI_08M07_melon07_13091 (1/36) ...
NAME = 07.HU1.1.1309.1
OK
```

```
-----
BB_BBI_08M07_melon07_13092 (2/36) ...
NAME = 07.HU1.1.1309.2
OK
```

```
-----
BB_BBI_08M07_melon07_13101 (3/36) ...
NAME = 07.HU1.2.1310.1
OK
```

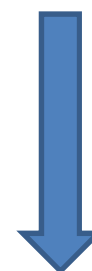
```
-----
BB_BBI_08M07_melon07_13102 (4/36) ...
NAME = 07.HU1.2.1310.2
OK
```

...

```
-----
BB_BBI_08M07_melon07_13372 (34/36) ...
NAME = 07.HU3.5.1337.2
OK
```

```
-----
BB_BBI_08M07_melon07_13381 (35/36) ...
NAME = 07.HU3.6.1338.1
OK
```

```
-----
BB_BBI_08M07_melon07_13382 (36/36) ...
NAME = 07.HU3.6.1338.2
OK
Pack ...OK
```



```
[djacob@proticdb nmrview]$ ll ./data/HUG007/procs/
total 9756
-rw-r--r-- 1 djacob users      28 Mar 26 15:03 factors
lrwxrwxrwx 1 djacob users      11 Mar 26 15:03 rawfile -> samples.csv
-rw-r--r-- 1 djacob users    1812 Mar 26 15:03 samples.csv
-rw-r--r-- 1 djacob users 9961496 Mar 26 15:04 specs.pack
```

Step 3: configuration file : ./etc/nmrproc.conf

[GLOBAL]

Declaration of global variables

Warning: Take care not putting spaces each side of equal sign, in order to be executed as a script shell

VARNAME=anything including spaces

DEBUG=0

The root of the bulk of your installation.

ROOTDIR=/mnt/var/sys/projets/nmrview

The root of the datasets

DATASETS=/mnt/var/sys/projets/nmrview/data

BASEURL=www.cbib.u-bordeaux2.fr

URLROOT=/SPECNMR

jQuery UI plugin : simple.html

```
<!DOCTYPE html PUBLIC "-//W3C//DTD XHTML 1.0 Strict//EN" "http://www.w3.org/TR/xhtml1/DTD/xhtml1-strict.dtd">
<html xmlns="http://www.w3.org/1999/xhtml" xml:lang="en" lang="en">
<head>
  <meta charset="utf-8" />
  <TITLE>NMRProcFlow - Viewer</TITLE>
  <link rel="stylesheet" href="/SPECNMR/css/redmond/jquery-ui.min.css">
  <script src="http://code.jquery.com/jquery-1.9.1.js"></script>
  <script src="http://code.jquery.com/ui/1.10.0/jquery-ui.js"></script>
  <script src="/SPECNMR/js/ui.nmrview.js"></script>
  <script>
    $(function() {
      $( "#nmrview" ).nmrview({
        url: '/SPECNMR/view', dataset: 'HUG007', colorby: 0, width: 'auto'
      }).show();
    });
  </script>
</head>
<body>
  <div id="nmrview"></div>
</body>
</html>
```

