

Conñjur

An Open Source Solution for NMR Software Integration

2012 CT NMR Workshop Day 1

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Acknowledgements



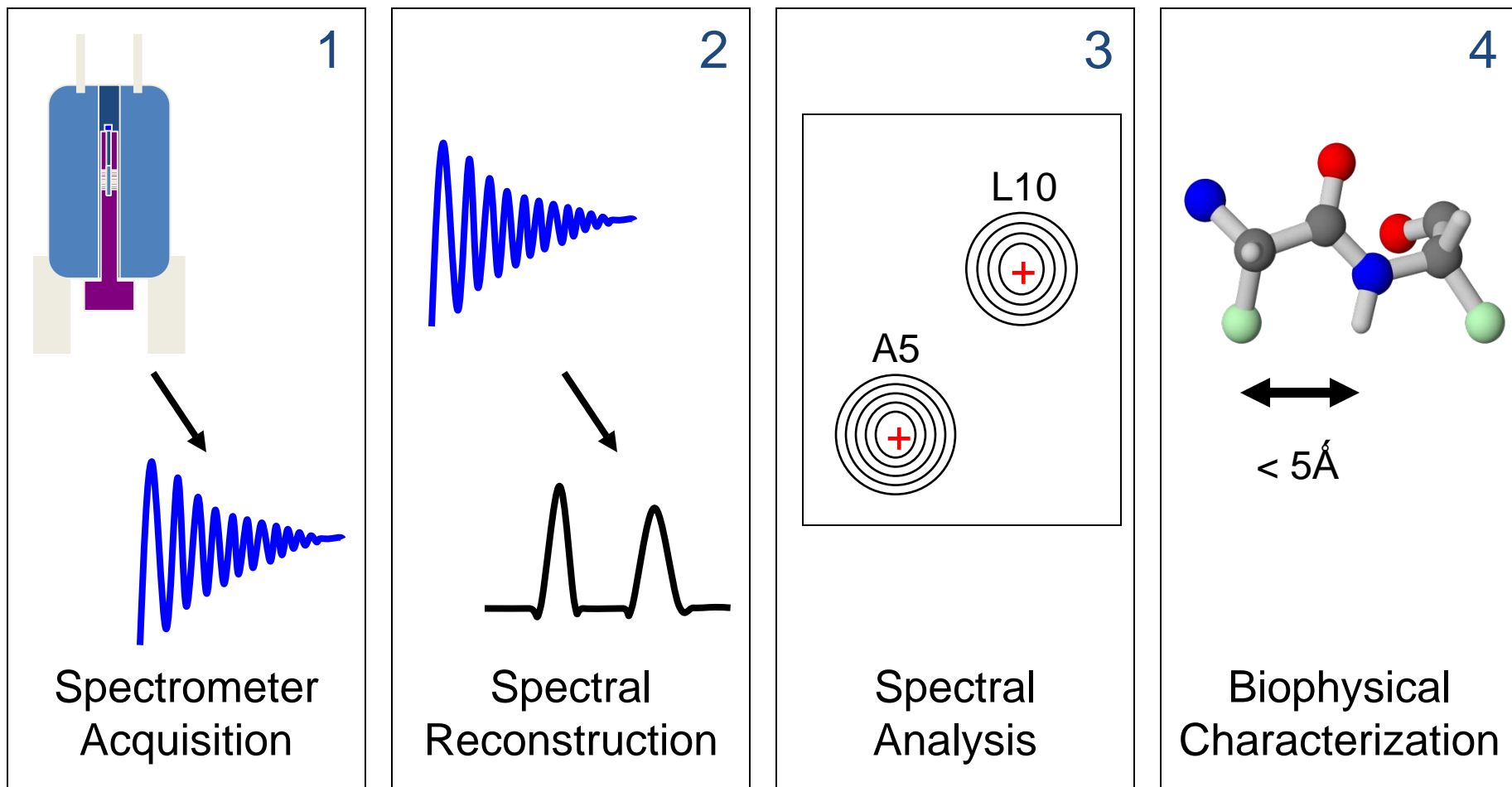
Matthew Fenwick
Jeffrey C. Hoch
Mark W. Maciejewski
Mehdi Mobli
RJ Nowling
Colbert Sesanker
Jay Vyas



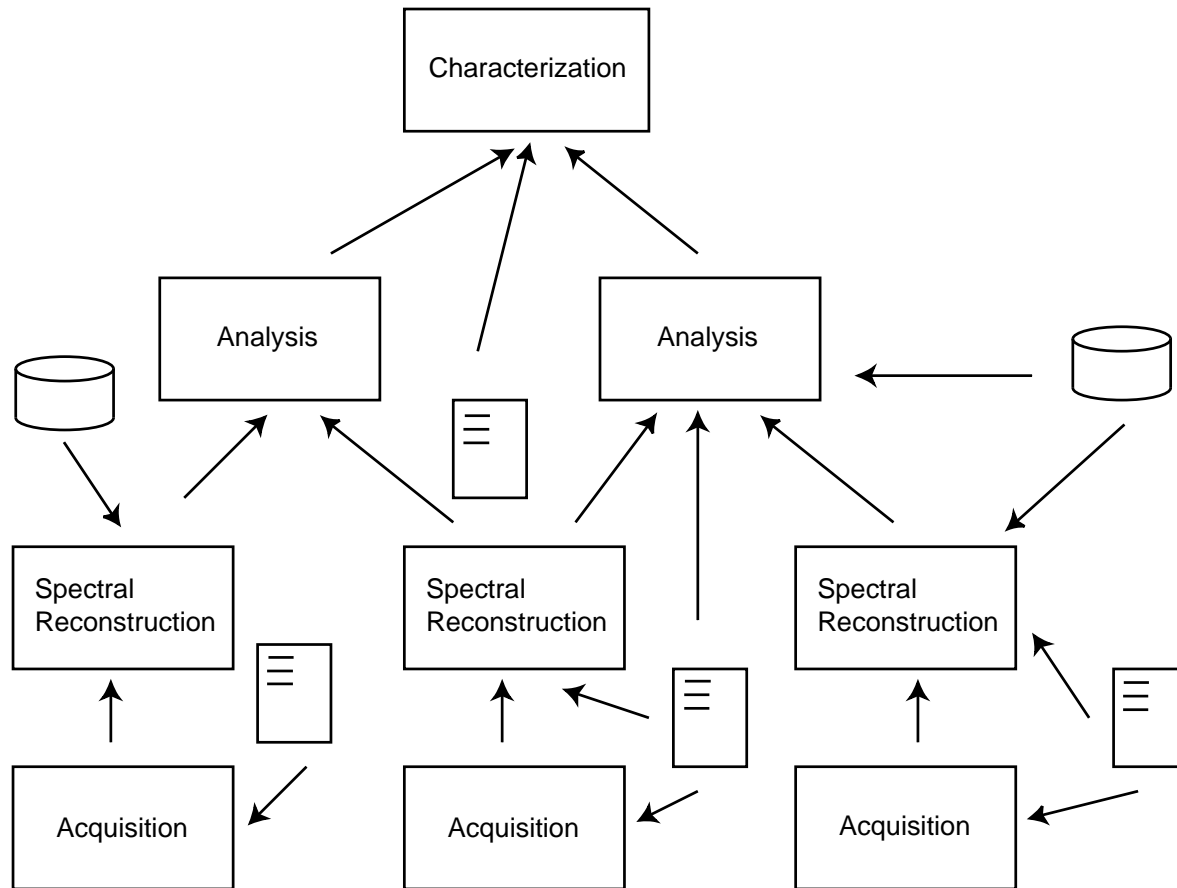
Heidi J.C. Ellis
Gerard Weatherby
Rensselaer at Hartford:
Timothy O. Martyn
NIDDK: Frank Delaglio
Rowland Institute: Alan Stern



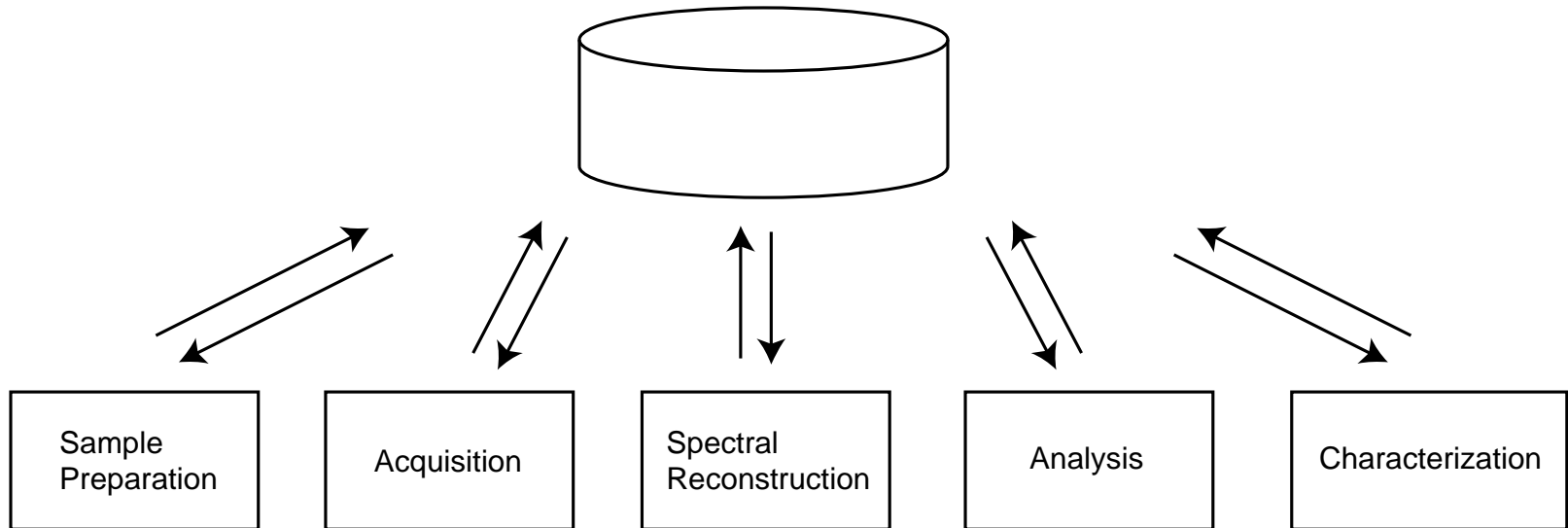
NMR Computational Pipeline



Current Data Flow



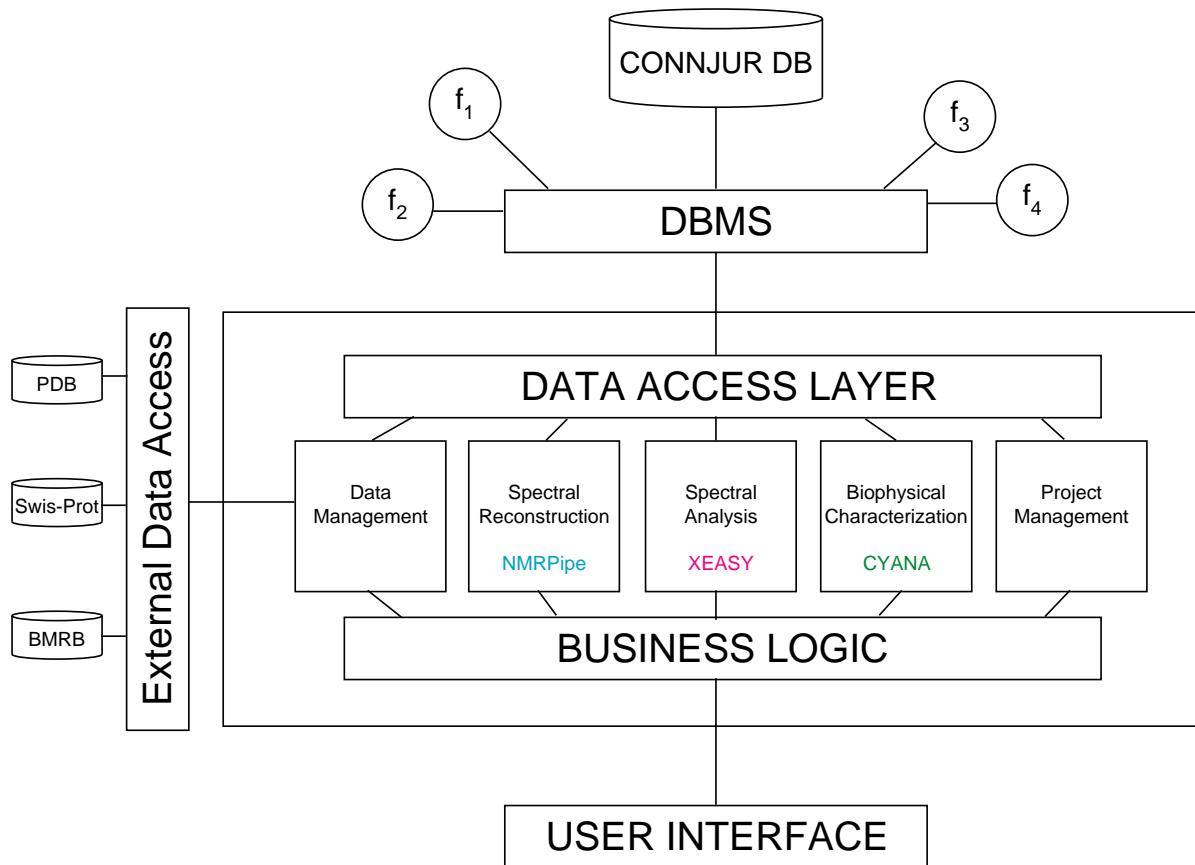
CONNJUR Data Flow



CONNJUR Software

- Connjur will provide the interface between existing software tools and a relational database
- Existing software tools have extensive history and are time-tested
- User interface is designed to aid in navigation and management

3-Tier Architecture



Free and Open Source

- Price: Free to download and install
- Extensibility: No restrictions or royalties to modify or resell
- Transparency: Source code readily inspected and verified
- Active Development: the scientific community is encouraged to aid in the development of CONNJUR
- Perpetual: If we are unable to continue the project, anyone is free to continue developing

Free/Open Source Interoperability

- Operating System: LINUX
- Framework Language: JAVA
- Relational Database: MySQL

bash vs. csh – the shell wars

= comment

#!/bin/csh

which nmrPipe tool? nmrPipe,
var2pipe, xyz2pipe, etc.

My Processing Script

nmrPipe -in mydata.pipe \

| nmrPipe -fn SOL -mode 1 -fl 16 -fs 1 -poly \

| nmrPipe -fn CBF -last 12 \

| nmrPipe -fn GMB -lb -7 -gb 0.1 -size 512 -c 0.5 \

| nmrPipe -fn ZF -size 2048 \

| nmrPipe -fn FT -verb \

| nmrPipe -fn PS -p0 68.6 -p1 -34.8 -di \

| nmrPipe -fn EXT -left -sw -verb \

| nmrPipe -fn TP \

| nmrPipe -fn LP -fb -ord 30 -x1 2 -xn 128 -pred 64 -fix -fixMode 1 -after \

| nmrPipe -fn SP -off 0.39 -end 0.98 -pow 2 -size 192 -c 0.5 \

| nmrPipe -fn ZF -size 256 \

| nmrPipe -fn FT -verb \

| nmrPipe -fn PS -p0 9.0 -p1 20.0 -di \

-out mydata.ft2 -ov

watch for trailing spaces!

Syntax?

filenames and filesystems

How much of the above information is NMR related?

How much is related to nmrPipe or the computer we are using?

Functionality and Function Order!

```
#!/bin/csh

# My Processing Script
nmrPipe -in mydata.pipe \
| nmrPipe -fn SOL -mode 1 -fl 16 -fs 1 -poly \
| nmrPipe -fn CBF -last 12 \
| nmrPipe -fn GMB -lb -7 -gb 0.1 -size 512 -c 0.5 \
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| nmrPipe -fn FT -verb \
| nmrPipe -fn PS -p0 -9.0 -p1 20.0 -di \
-out mydata.ft2 -ov
```

What procedures do we use to massage our data?

What procedures do we use to transform our data?