

Compilació dels programes AU

Aquesta part és tan llarga i específica que s'ha mogut a una pàgina a part.

Al procés de configuració del TopSpin vaig deixar per més endavant la compilació dels programes AU

-  `cplbruk all` per compilar tots els programes AU de Bruker.
-  `cpluser all` per compilar tots els programes AU dels usuaris.

però alguns d'aquests programes són necessaris per adquirir espectres i no puc comprovar el funcionament del programa i espectròmetre fins completar aquest pas.

Registres a la Bruker Knowledge Base relacionat amb la compilació de programes AU

A la base de dades Bruker Knowledge Base hi ha dos registres relacionats amb la compilació de programes AU,

- [Item#: 9577. With TopSpin 1.3pl10 it is not possible to compile AU programs under CentOS5 \(or RedHat Enterprise Linux 5\)](#)
- [Item#: 9641. Some AU programs do not compile with native compiler](#)

Primer intent de compilació

Executo la comanda `cplbruk` per compilar programes AU de Bruker i provo a compilar el programa `df1shift` però dóna el següent error,

```
/opt/topspin1.3/gnu/bin/./lib/gcc-lib/i686-pc-linux-gnu/3.3.5/./././././././i686-pc-linux-gnu/bin/ld: crt1.o: No such file: No such file or directory
collect2: ld returned 1 exit status
```

Aquest error està relacionat amb l'[Item #9557](#) esmentat més amunt, i per resoldre'l em descarrego la nova versió del programa `makeau`.

Per evitar altres problemes, també em descarrego les noves versions d'algunes programes AU disponibles a l'[Item #9641](#)

Segon intent de compilació

L'intent de compilació amb la nova versió del programa `makeau` tampoc funciona, però en aquest cas la solució és trivial: a la nova versió s'assumeix que el directori d'instal·lació del TopSpin és `/opt/topspin` mentre que en el nostre cas és `/opt/topspin1.3`. L'error es resol editant la primera línia del programa `makeau`,

```
# diff makeau makeau.BKUP-20150923
1c1
< #! /opt/topspin1.3/perl/bin/perl -I/opt/topspin1.3/perl/lib/perl5
---
> #! /opt/topspin/perl/bin/perl -I/opt/topspin/perl/lib/perl5
```

Per altra banda, per tenir més informació sobre el procés de compilació, decideixo executar el programa makeau directament des d'una terminal i no des de dins del TopSpin. Per això cal definir algunes variables d'entorn,

```
# export XWINNMRHOME=/opt/topspin1.3
# export PATH=$PATH:/opt/topspin1.3/gnu/bin/
# export LD_LIBRARY_PATH=/usr/lib32
# export LIBRARY_PATH=/usr/lib32:$LIBRARY_PATH

# printenv LIBRARY_PATH LD_LIBRARY_PATH XWINNMRHOME PATH
/usr/lib32:
/usr/lib32
/opt/topspin1.3
/usr/local/sbin:/usr/local/bin:/usr/sbin:/usr/bin:/sbin:/bin:/opt/topspin1.3
/gnu/bin/
```

Un cop definides aquestes variables, torno a executar el programa, però encara no aconseguiré compilar el programa i dona el següent error,

```
# ./makeau -show -verbose au_zg
makeau ($Revision: 1.108.2.2 $ )
  OperatingSystem=LINUX
Using GNU Compiler /opt/topspin1.3/gnu/bin/gcc and
/opt/topspin1.3/gnu/bin/c++
Setup for native compiler
  CC=gcc
  LD=c++
:
/opt/topspin1.3/gnu/bin/../../lib/gcc-lib/i686-pc-linux-
gnu/3.3.5/../../../../../i686-pc-linux-gnu/bin/ld:/usr/lib32/libc.so: file
format not recognized; treating as linker script
/opt/topspin1.3/gnu/bin/../../lib/gcc-lib/i686-pc-linux-
gnu/3.3.5/../../../../../i686-pc-linux-gnu/bin/ld:/usr/lib32/libc.so:5: parse
error
collect2: ld returned 1 exit status
exit status is: 256 1
```

Provo el suggeriment que trobo [aquí](#) i [aquí](#), i faig el següent canvi al fitxer `/usr/lib32/libc.so`

```
# diff libc.so libc.so.BKUP-20150924
5c5
< GROUP ( /lib32/libc.so.6 /usr/lib32/libc_nonshared.a )
---
```

```
> GROUP ( /lib32/libc.so.6 /usr/lib32/libc_nonshared.a AS_NEEDED (
/lib32/ld-linux.so.2 ) )
```

Llavors, finalment aconseguixo compilar el programa au_zg,

```
# ./makeau -show -verbose au_zg
makeau ($Revision: 1.108.2.2 $ )
  OperatingSystem=LINUX
Using GNU Compiler /opt/topspin1.3/gnu/bin/gcc and
/opt/topspin1.3/gnu/bin/c++
Setup for native compiler
  CC=gcc
  LD=c++

Installed RPM packages:
Can't exec "rpm": No such file or directory at ./makeau line 312.

used kernel release: 3.2.0-4-amd64
Known paths:
Known paths:
.
/usr/local/sbin
/usr/local/bin
/usr/sbin
/usr/bin
/sbin
/bin
/opt/topspin1.3/gnu/bin/
/opt/topspin1.3/prog/bin
Current environment:
HOME=/root
XAUTHORITY=/var/run/gdm3/auth-for-sermnadmin-MBTzen/database
SUDO_GID=1000
LD_LIBRARY_PATH=/usr/lib32:/lib32
DISPLAY=:0
LIBRARY_PATH=/usr/lib32
_RLD_ARGS=-ignore_unresolved
MAIL=/var/mail/root
PWD=/opt/topspin1.3/exp/stan/nmr/au
LANG=en_US.utf8
USER=root
XWINNMHOME=/opt/topspin1.3
LOGNAME=root
USERNAME=root
SHLVL=1
OLDPWD=/opt/topspin1.3/exp/stan/nmr
_=./makeau
PATH=./usr/local/sbin:/usr/local/bin:/usr/sbin:/usr/bin:/sbin:/bin:/opt/top
spin1.3/gnu/bin:/opt/topspin1.3/prog/bin
COLORTERM=gnome-terminal
SUDO_USER=sermnadmin
```

```
LS_COLORS=rs=0:di=01;34:ln=01;36:mh=00:pi=40;33:so=01;35:do=01;35:bd=40;33;0
1:cd=40;33;01:or=40;31;01:su=37;41:sg=30;43:ca=30;4
1:tw=30;42:ow=34;42:st=37;44:ex=01;32:*.tar=01;31:*.tgz=01;31:*.arj=01;31:*.
taz=01;31:*.lzh=01;31:*.lzma=01;31:*.tlz=01;31:*.txz=
01;31:*.zip=01;31:*.z=01;31:*.Z=01;31:*.dz=01;31:*.gz=01;31:*.lz=01;31:*.xz=
01;31:*.bz2=01;31:*.bz=01;31:*.tbz=01;31:*.tbz2=01;31
:*.tz=01;31:*.deb=01;31:*.rpm=01;31:*.jar=01;31:*.war=01;31:*.ear=01;31:*.sa
r=01;31:*.rar=01;31:*.ace=01;31:*.zoo=01;31:*.cpio=01
;31:*.7z=01;31:*.rz=01;31:*.jpg=01;35:*.jpeg=01;35:*.gif=01;35:*.bmp=01;35:*
.pbm=01;35:*.pgm=01;35:*.ppm=01;35:*.tga=01;35:*.xbm=
01;35:*.xpm=01;35:*.tif=01;35:*.tiff=01;35:*.png=01;35:*.svg=01;35:*.svgz=01
;35:*.mng=01;35:*.pcx=01;35:*.mov=01;35:*.mpg=01;35:*
.mpeg=01;35:*.m2v=01;35:*.mkv=01;35:*.webm=01;35:*.ogm=01;35:*.mp4=01;35:*.m
4v=01;35:*.mp4v=01;35:*.vob=01;35:*.qt=01;35:*.nuv=01
;35:*.wmv=01;35:*.asf=01;35:*.rm=01;35:*.rmvb=01;35:*.flc=01;35:*.avi=01;35:
*.fli=01;35:*.flv=01;35:*.gl=01;35:*.dl=01;35:*.xcf=0
1;35:*.xwd=01;35:*.yuv=01;35:*.cgm=01;35:*.emf=01;35:*.axv=01;35:*.anx=01;35
:*.ogv=01;35:*.ogx=01;35:*.aac=00;36:*.au=00;36:*.fla
c=00;36:*.mid=00;36:*.midi=00;36:*.mka=00;36:*.mp3=00;36:*.mpc=00;36:*.ogg=0
0;36:*.ra=00;36:*.wav=00;36:*.axa=00;36:*.oga=00;36:*
.spx=00;36:*.xspf=00;36:
SHELL=/bin/bash
TERM=screen
SUDO_COMMAND=/bin/bash
SUDO_UID=1000
LibraryExtension: .so
StaticLibraryExtension: .a
SharedLibraryExtension: .so
LibraryPath: shlib
StaticLibraryPath: lib
SharedLibraryPath: shlib
ObjectExtension: .o
BinaryExtension:
BinaryExtension:
Check for /opt/topspin1.3/exp/stan/nmr/au/paravision_1.3.pl
Check for /opt/topspin1.3/exp/stan/nmr/au/user_1.3.pl
submacro(/opt/topspin1.3/prog/include/inc
/opt/topspin1.3/exp/stan/nmr/au/src/au_zg
/opt/topspin1.3/prog/au/bin/au_zg.E)
No INC_FLAGS found: using default library list
Used libraries:
    auliba
    aulibp
    chparmod
    sxutil
    libhpcu
    libBpsu
    ConvSf
    libSwish
    libVtu
```

```
lib_sbsb
lib_tty
librrs
liblrs
Bis
convpw
editpar
libacq
util
aulibp
uni
par
libPath
libcb
libUtil
libCUtil
libShapeIO
libFunc
libJCamp
libCt
libQTP
```

Included Libraries

```
auliba.so
aulibp.so
chparmod.so
sxutil.so
libhpcu.so
libBpsu.so
ConvSf.so
libSwish.so
libVtu.so
lib_sbsb.so
lib_tty.so
librrs.so
liblrs.so
Bis.so
convpw.so
editpar.so
libacq.so
util.so
aulibp.so
uni.so
par.so
libPath.so
libcb.so
libUtil.so
libCUtil.so
libShapeIO.so
libFunc.so
libJCamp.so
libCt.so
```

```
libQTP.so
autila.a
autilbp.a
chparmod.a
libacq.a
editpar.a
util.a
uni.a
libPath.a
libcb.a
```

```
Combine /opt/topspin1.3/exp/stan/nmr/au/vorspann
/opt/topspin1.3/prog/au/bin/au_zg.E > /opt/topspin1.3/prog/au/bin/au_zg.c
```

```
Include Option: -I/opt/topspin1.3/prog/include
```

```
chdir /opt/topspin1.3/prog/au/bin
```

```
Opsys=LINUX
```

```
gcc -c -DLINUX_INTEL -D_REENTRANT -D_FILE_OFFSET_BITS=64 -D_LARGEFILE_SOURCE
-g -m32 -w -v -I/opt/topspin1.3/prog/include au_zg
.c
```

```
Using built-in specs.
```

```
COLLECT_GCC=gcc
```

```
Target: x86_64-linux-gnu
```

```
Configured with: ../src/configure -v --with-pkgversion='Debian 4.7.2-5' --
with-bugurl=file:///usr/share/doc/gcc-4.7/README.Bugs -
-enable-languages=c,c++,go,fortran,objc,obj-c++ --prefix=/usr --program-
suffix=-4.7 --enable-shared --enable-linker-build-id --wi
th-system-zlib --libexecdir=/usr/lib --without-included-gettext --enable-
threads=posix --with-gxx-include-dir=/usr/include/c++/4.
7 --libdir=/usr/lib --enable-nls --with-sysroot=/ --enable-clocale=gnu --
enable-libstdcxx-debug --enable-libstdcxx-time=yes --ena
ble-gnu-unique-object --enable-plugin --enable-objc-gc --with-arch-32=i586 -
-with-tune=generic --enable-checking=release --build=
x86_64-linux-gnu --host=x86_64-linux-gnu --target=x86_64-linux-gnu
```

```
Thread model: posix
```

```
gcc version 4.7.2 (Debian 4.7.2-5)
```

```
COLLECT_GCC_OPTIONS='-c' '-D' 'LINUX_INTEL' '-D' '_REENTRANT' '-D'
'_FILE_OFFSET_BITS=64' '-D' '_LARGEFILE_SOURCE' '-g' '-m32' '-
w' '-v' '-I' '/opt/topspin1.3/prog/include' '-mtune=generic' '-march=i586'
/usr/lib/gcc/x86_64-linux-gnu/4.7/cc1 -quiet -v -I
/opt/topspin1.3/prog/include -imultilib 32 -imultiarch i386-linux-gnu -D
LINU
```

```
X_INTEL -D _REENTRANT -D _FILE_OFFSET_BITS=64 -D _LARGEFILE_SOURCE au_zg.c -
quiet -dumpbase au_zg.c -m32 -mtune=generic -march=i5
```

```
86 -auxbase au_zg -g -w -version -o /tmp/cc4rFa4B.s
```

```
GNU C (Debian 4.7.2-5) version 4.7.2 (x86_64-linux-gnu)
```

```
compiled by GNU C version 4.7.2, GMP version 5.0.5, MPFR version
3.1.0-p10, MPC version 0.9
```

```
GGC heuristics: --param ggc-min-expand=100 --param ggc-min-heapsize=131072
ignoring nonexistent directory "/usr/local/include/i386-linux-gnu"
```

```

ignoring nonexistent directory "/usr/lib/gcc/x86_64-linux-
gnu/4.7/../../../../x86_64-linux-gnu/include"
ignoring nonexistent directory "/usr/include/i386-linux-gnu"
#include "... search starts here:
#include <...> search starts here:
/opt/topspin1.3/prog/include
/usr/lib/gcc/x86_64-linux-gnu/4.7/include
/usr/local/include
/usr/lib/gcc/x86_64-linux-gnu/4.7/include-fixed
/usr/include
End of search list.
GNU C (Debian 4.7.2-5) version 4.7.2 (x86_64-linux-gnu)
    compiled by GNU C version 4.7.2, GMP version 5.0.5, MPFR version
3.1.0-p10, MPC version 0.9
GGC heuristics: --param ggc-min-expand=100 --param ggc-min-heapsize=131072
Compiler executable checksum: 7fa7c2a970be5e19ce72b2057c14800d
COLLECT_GCC_OPTIONS='-c' '-D' 'LINUX_INTEL' '-D' '_REENTRANT' '-D'
'_FILE_OFFSET_BITS=64' '-D' '_LARGEFILE_SOURCE' '-g' '-m32' '-
w' '-v' '-I' '/opt/topspin1.3/prog/include' '-mtune=generic' '-march=i586'
as -v -W -I /opt/topspin1.3/prog/include --32 -o au_zg.o /tmp/cc4rFa4B.s
GNU assembler version 2.22 (x86_64-linux-gnu) using BFD version (GNU
Binutils for Debian) 2.22
COMPILER_PATH=/usr/lib/gcc/x86_64-linux-gnu/4.7:/usr/lib/gcc/x86_64-linux-
gnu/4.7:/usr/lib/gcc/x86_64-linux-gnu:/usr/lib/gcc/x
86_64-linux-gnu/4.7:/usr/lib/gcc/x86_64-linux-gnu/
LIBRARY_PATH=/usr/lib32/./lib32:/usr/lib/gcc/x86_64-linux-
gnu/4.7/32:/usr/lib/gcc/x86_64-linux-gnu/4.7/../../../../i386-linux-gnu
:/usr/lib/gcc/x86_64-linux-gnu/4.7/../../../../lib32:/lib/i386-linux-
gnu:/lib/./lib32:/usr/lib/i386-linux-gnu:/usr/lib/./l
ib32:/usr/lib32:/usr/lib/gcc/x86_64-linux-gnu/4.7:/usr/lib/gcc/x86_64-
linux-gnu/4.7/../../../../i386-linux-gnu:/usr/lib/gcc/x86_
64-linux-gnu/4.7/../../../../lib/i386-linux-gnu:/lib:/usr/lib/i386-linux-
gnu:/usr/lib/
COLLECT_GCC_OPTIONS='-c' '-D' 'LINUX_INTEL' '-D' '_REENTRANT' '-D'
'_FILE_OFFSET_BITS=64' '-D' '_LARGEFILE_SOURCE' '-g' '-m32' '-
w' '-v' '-I' '/opt/topspin1.3/prog/include' '-mtune=generic' '-march=i586'
exit=0 sig=0 dump=0
Used Libraries
auliba.so aulibp.so chparmod.so sxutil.so libhpcu.so libBpsu.so ConvSf.so
libSwish.so libVtu.so lib_sbsb.so lib_tty.so librrs.so
liblrs.so Bis.so convpw.so editpar.so libacq.so util.so aulibp.so uni.so
par.so libPath.so libcb.so libUtil.so libCUtil.so libSha
peIO.so libFunc.so libJCamp.so libCt.so libQTP.so auliba.a aulibp.a
chparmod.a libacq.a editpar.a util.a uni.a par.a libPath.a li
bcb.a
c++ -m32 -Wl,-warn-common,-warn-constructors -L/opt/topspin1.3/prog/shlib -
lstdc++ -v -s /opt/topspin1.3/prog/au/bin/au_zg.o
/opt/topspin1.3/prog/shlib/auliba.so /opt/topspin1.3/prog/shlib/aulibp.so
/opt/topspin1.3/prog/shlib/chparmod.so /opt/topspin1.3/
prog/shlib/sxutil.so /opt/topspin1.3/prog/shlib/libhpcu.so
/opt/topspin1.3/prog/shlib/libBpsu.so /opt/topspin1.3/prog/shlib/ConvS

```

```
f.so /opt/topspin1.3/prog/shlib/libSwish.so
/opt/topspin1.3/prog/shlib/libVtu.so /opt/topspin1.3/prog/shlib/lib_sbsb.so
/opt/tops
pin1.3/prog/shlib/lib_tty.so /opt/topspin1.3/prog/shlib/librrs.so
/opt/topspin1.3/prog/shlib/liblrs.so /opt/topspin1.3/prog/shlib
/Bis.so /opt/topspin1.3/prog/shlib/convpw.so
/opt/topspin1.3/prog/shlib/editpar.so /opt/topspin1.3/prog/shlib/libacq.so
/opt/tops
pin1.3/prog/shlib/util.so /opt/topspin1.3/prog/shlib/aulibp.so
/opt/topspin1.3/prog/shlib/uni.so /opt/topspin1.3/prog/shlib/par.s
o /opt/topspin1.3/prog/shlib/libPath.so /opt/topspin1.3/prog/shlib/libcb.so
/opt/topspin1.3/prog/shlib/libUtil.so /opt/topspin1.3
/prog/shlib/libCUtil.so /opt/topspin1.3/prog/shlib/libShapeI0.so
/opt/topspin1.3/prog/shlib/libFunc.so /opt/topspin1.3/prog/shlib
/libJCamp.so /opt/topspin1.3/prog/shlib/libCt.so
/opt/topspin1.3/prog/shlib/libQTP.so /opt/topspin1.3/prog/lib/auliba.a
/opt/tops
pin1.3/prog/lib/aulibp.a /opt/topspin1.3/prog/lib/chparamod.a
/opt/topspin1.3/prog/lib/libacq.a /opt/topspin1.3/prog/lib/editpar.a
/opt/topspin1.3/prog/lib/util.a /opt/topspin1.3/prog/lib/uni.a
/opt/topspin1.3/prog/lib/par.a /opt/topspin1.3/prog/lib/libPath.a
/opt/topspin1.3/prog/lib/libcb.a -lm -ldl -o au_zg
c++ -m32 -Wl,-warn-common,-warn-constructors -L/opt/topspin1.3/prog/shlib -
lstdc++ -v -s /opt/topspin1.3/prog/au/bin/au_zg.o
/opt/topspin1.3/prog/shlib/auliba.so /opt/topspin1.3/prog/shlib/aulibp.so
/opt/topspin1.3/prog/shlib/chparamod.so /opt/topspin1.3/
prog/shlib/sxutil.so /opt/topspin1.3/prog/shlib/libhpcu.so
/opt/topspin1.3/prog/shlib/libBpsu.so /opt/topspin1.3/prog/shlib/ConvS
f.so /opt/topspin1.3/prog/shlib/libSwish.so
/opt/topspin1.3/prog/shlib/libVtu.so /opt/topspin1.3/prog/shlib/lib_sbsb.so
/opt/tops
pin1.3/prog/shlib/lib_tty.so /opt/topspin1.3/prog/shlib/librrs.so
/opt/topspin1.3/prog/shlib/liblrs.so /opt/topspin1.3/prog/shlib
/Bis.so /opt/topspin1.3/prog/shlib/convpw.so
/opt/topspin1.3/prog/shlib/editpar.so /opt/topspin1.3/prog/shlib/libacq.so
/opt/tops
pin1.3/prog/shlib/util.so /opt/topspin1.3/prog/shlib/aulibp.so
/opt/topspin1.3/prog/shlib/uni.so /opt/topspin1.3/prog/shlib/par.s
o /opt/topspin1.3/prog/shlib/libPath.so /opt/topspin1.3/prog/shlib/libcb.so
/opt/topspin1.3/prog/shlib/libUtil.so /opt/topspin1.3
/prog/shlib/libCUtil.so /opt/topspin1.3/prog/shlib/libShapeI0.so
/opt/topspin1.3/prog/shlib/libFunc.so /opt/topspin1.3/prog/shlib
/libJCamp.so /opt/topspin1.3/prog/shlib/libCt.so
/opt/topspin1.3/prog/shlib/libQTP.so /opt/topspin1.3/prog/lib/auliba.a
/opt/tops
pin1.3/prog/lib/aulibp.a /opt/topspin1.3/prog/lib/chparamod.a
/opt/topspin1.3/prog/lib/libacq.a /opt/topspin1.3/prog/lib/editpar.a
/opt/topspin1.3/prog/lib/util.a /opt/topspin1.3/prog/lib/uni.a
/opt/topspin1.3/prog/lib/par.a /opt/topspin1.3/prog/lib/libPath.a
/opt/topspin1.3/prog/lib/libcb.a -lm -ldl -o au_zg
```

```

Reading specs from /opt/topspin1.3/gnu/bin/./lib/gcc-lib/i686-pc-linux-
gnu/3.3.5/specs
Configured with: ../gcc-3.3.5/configure --prefix=/pr/gnu --enable-
threads=posix --enable-__cxa_atexit --enable-languages=c,c++ --
with-cpu=pentium4
Thread model: posix
gcc version 3.3.5
/opt/topspin1.3/gnu/bin/./lib/gcc-lib/i686-pc-linux-gnu/3.3.5/collect2 --
eh-frame-hdr -m elf_i386 -dynamic-linker /lib/ld-linux
.so.2 -o au_zg -s /usr/lib32/crt1.o /usr/lib32/crti.o
/opt/topspin1.3/gnu/bin/./lib/gcc-lib/i686-pc-linux-gnu/3.3.5/crtbegin.o -
L/opt/topspin1.3/prog/shlib -L/opt/topspin1.3/gnu/bin/./lib/gcc-lib/i686-
pc-linux-gnu/3.3.5 -L/opt/topspin1.3/gnu/bin/./lib/gcc
-lib -L/usr/lib32 -L/opt/topspin1.3/gnu/bin/./lib/gcc-lib/i686-pc-linux-
gnu/3.3.5/././././././i686-pc-linux-gnu/lib -L/opt/topsp
in1.3/gnu/bin/./lib/gcc-lib/i686-pc-linux-gnu/3.3.5/./././.. -warn-common -
warn-constructors -lstdc++ /opt/topspin1.3/prog/au/bi
n/au_zg.o /opt/topspin1.3/prog/shlib/auliba.so
/opt/topspin1.3/prog/shlib/aulibp.so /opt/topspin1.3/prog/shlib/chparmod.so
/opt/t
opspin1.3/prog/shlib/sxutil.so /opt/topspin1.3/prog/shlib/libhpcu.so
/opt/topspin1.3/prog/shlib/libBpsu.so /opt/topspin1.3/prog/s
hlib/ConvSf.so /opt/topspin1.3/prog/shlib/libSwish.so
/opt/topspin1.3/prog/shlib/libVtu.so /opt/topspin1.3/prog/shlib/lib_sbsb.so
/opt/topspin1.3/prog/shlib/lib_tty.so /opt/topspin1.3/prog/shlib/librrs.so
/opt/topspin1.3/prog/shlib/liblrs.so /opt/topspin1.3/
prog/shlib/Bis.so /opt/topspin1.3/prog/shlib/convpw.so
/opt/topspin1.3/prog/shlib/editpar.so /opt/topspin1.3/prog/shlib/libacq.so
/opt/topspin1.3/prog/shlib/util.so /opt/topspin1.3/prog/shlib/aulibp.so
/opt/topspin1.3/prog/shlib/uni.so /opt/topspin1.3/prog/s
hlib/par.so /opt/topspin1.3/prog/shlib/libPath.so
/opt/topspin1.3/prog/shlib/libcb.so /opt/topspin1.3/prog/shlib/libUtil.so
/opt/
topspin1.3/prog/shlib/libCUtil.so /opt/topspin1.3/prog/shlib/libShapeIO.so
/opt/topspin1.3/prog/shlib/libFunc.so /opt/topspin1.3/
prog/shlib/libJCamp.so /opt/topspin1.3/prog/shlib/libCt.so
/opt/topspin1.3/prog/shlib/libQTP.so /opt/topspin1.3/prog/lib/auliba.a
/opt/topspin1.3/prog/lib/aulibp.a /opt/topspin1.3/prog/lib/chparmod.a
/opt/topspin1.3/prog/lib/libacq.a /opt/topspin1.3/prog/lib
/editpar.a /opt/topspin1.3/prog/lib/util.a /opt/topspin1.3/prog/lib/uni.a
/opt/topspin1.3/prog/lib/par.a /opt/topspin1.3/prog/lib
/libPath.a /opt/topspin1.3/prog/lib/libcb.a -ldl -lstdc++ -lm -lgcc_s -lgcc
-lc -lgcc_s -lgcc /opt/topspin1.3/gnu/bin/./lib/gcc-
lib/i686-pc-linux-gnu/3.3.5/crtend.o /usr/lib32/crtn.o
exit status is: 0 0

```

i quan comprovo el fitxer creat trobo que és un executable de 32-bits

```

# file /opt/topspin1.3/prog/au/bin/au_zg
/opt/topspin1.3/prog/au/bin/au_zg: ELF 32-bit LSB executable, Intel 80386,
version 1 (SYSV), dynamically linked (uses shared libs), for GNU/Linux

```

2.6.26, stripped

i si afegim a la variable `LD_LIBRARY_PATH` les carpetes definides a l'entorn d'execució del TopSpin (veure fitxer `/opt/topspin1.3/prog/bin/topspin`)

```
export
```

```
LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/opt/topspin1.3/prog/pvshlib:/opt/topspin1.3/prog/shlib
```

el programa `ldd` ens mostra que totes les biblioteques emprades pel programa `au_zg` estan disponibles,

```
# ldd /opt/topspin1.3/prog/au/bin/au_zg
linux-gate.so.1 => (0xf77e0000)
libstdc++.so.5 => /opt/topspin1.3/prog/shlib/libstdc++.so.5
(0xf7723000)
auliba.so => /opt/topspin1.3/prog/shlib/auliba.so (0xf76ed000)
aulibp.so => /opt/topspin1.3/prog/shlib/aulibp.so (0xf76df000)
chparmod.so => /opt/topspin1.3/prog/shlib/chparmod.so (0xf76d7000)
sxutil.so => /opt/topspin1.3/prog/shlib/sxutil.so (0xf7681000)
libhpcu.so => /opt/topspin1.3/prog/shlib/libhpcu.so (0xf7671000)
libBpsu.so => /opt/topspin1.3/prog/shlib/libBpsu.so (0xf7666000)
ConvSf.so => /opt/topspin1.3/prog/shlib/ConvSf.so (0xf7660000)
libSwish.so => /opt/topspin1.3/prog/shlib/libSwish.so (0xf7657000)
libVtu.so => /opt/topspin1.3/prog/shlib/libVtu.so (0xf764e000)
lib_sbsb.so => /opt/topspin1.3/prog/shlib/lib_sbsb.so (0xf763a000)
lib_tty.so => /opt/topspin1.3/prog/shlib/lib_tty.so (0xf762a000)
librrs.so => /opt/topspin1.3/prog/shlib/librrs.so (0xf7621000)
liblrs.so => /opt/topspin1.3/prog/shlib/liblrs.so (0xf761f000)
Bis.so => /opt/topspin1.3/prog/shlib/Bis.so (0xf75f5000)
convpw.so => /opt/topspin1.3/prog/shlib/convpw.so (0xf75ef000)
editpar.so => /opt/topspin1.3/prog/shlib/editpar.so (0xf757c000)
libacq.so => /opt/topspin1.3/prog/shlib/libacq.so (0xf754f000)
util.so => /opt/topspin1.3/prog/shlib/util.so (0xf7535000)
uni.so => /opt/topspin1.3/prog/shlib/uni.so (0xf7527000)
par.so => /opt/topspin1.3/prog/shlib/par.so (0xf751b000)
libPath.so => /opt/topspin1.3/prog/shlib/libPath.so (0xf7510000)
libcb.so => /opt/topspin1.3/prog/shlib/libcb.so (0xf7505000)
libUtil.so => /opt/topspin1.3/prog/shlib/libUtil.so (0xf74df000)
libCUtil.so => /opt/topspin1.3/prog/shlib/libCUtil.so (0xf74dd000)
libShapeIO.so => /opt/topspin1.3/prog/shlib/libShapeIO.so
(0xf74ca000)
libFunc.so => /opt/topspin1.3/prog/shlib/libFunc.so (0xf7491000)
libJCamp.so => /opt/topspin1.3/prog/shlib/libJCamp.so (0xf745e000)
libCt.so => /opt/topspin1.3/prog/shlib/libCt.so (0xf745a000)
libQTP.so => /opt/topspin1.3/prog/shlib/libQTP.so (0xf744c000)
libdl.so.2 => /lib32/libdl.so.2 (0xf7448000)
libm.so.6 => /lib32/libm.so.6 (0xf7422000)
libgcc_s.so.1 => /usr/lib32/libgcc_s.so.1 (0xf7404000)
libc.so.6 => /lib32/libc.so.6 (0xf729f000)
```

```
/lib/ld-linux.so.2 (0xf77e1000)
```

De totes formes, ara hauré d'esperar a tenir accés al TopSpin per poder comprovar si realment funciona el programa `au_zg` i l'adquisició d'espectres.

Canvis addicionals al programa 'makeau'

Per poder compilar els programes AU des de dins el TopSpin, caldrà comprovar si cal afegir al programa *makeau* les definicions de variables d'entorn

- `LD_LIBRARY_PATH=/usr/lib32`
- `LD_LIBRARY_PATH=/usr/lib32:$LD_LIBRARY_PATH`

o si n'hi ha prou amb definir-les al fitxer de configuració de l'entorn de l'usuari (fitxers `~/.bashrc` o `~/.bash_profile`).

Consultar:

- <http://tldp.org/HOWTO/Program-Library-HOWTO/shared-libraries.html>
- <https://wiki.debian.org/Multiarch/LibraryPathOverview>
- <http://askubuntu.com/questions/275965/how-to-list-all-variables-names-and-their-current-values/356973#356973>
 - hint: emprar la comanda `declare -xp` per veure les variables d'entorn definides a la sessió de Gnome.
- <http://askubuntu.com/questions/438150/scripts-in-etc-profile-d-being-ignored>
- <https://wiki.debian.org/EnvironmentVariables>
- <http://unix.stackexchange.com/questions/117467/how-to-permanently-set-environmental-variables>

Canvis al TopSpin

/opt/topspin1.3/prog/bin/topspin

Afegeixo la variable `$LD_LIBRARY_PATH` al final de la definició de la variable `LD_LIBRARY_PATH`,

```
# diff topspin topspin.ORIG-20150824
62c62
<     export
LD_LIBRARY_PATH="$szProgPath"/pvshlib:"$szProgPath"/shlib:$LD_LIBRARY_PATH
---
>     export LD_LIBRARY_PATH="$szProgPath"/pvshlib:"$szProgPath"/shlib
```

/etc/profile.d/topspin_compile_au.sh

Creo el fitxer `/etc/profile.d/topspin_compile_au.sh` que contindrà la definició de les variables d'entorn necessàries perquè funcioni la compilació dels programes AU,

```
# MCE - 20150925 - Library path environment variables added to allow  
# compiling TopSpin 1.3 AU programs in newer GNU/Linux versions
```

```
export PATH=$PATH:/opt/topspin1.3/gnu/bin  
export LIBRARY_PATH=/usr/lib32:$LIBRARY_PATH  
export LD_LIBRARY_PATH=/usr/lib32:/lib32:$LD_LIBRARY_PATH
```

Nova compilació dels programes AU

Executo la comanda `cplbruk all` per compilar tots els programes AU i els compila tots excepte els esmentats a l'item#: 9641. [Some AU programs do not compile with native compiler](#)

```
/opt/topspin1.3/exp/stan/nmr/au/src/coiltemp:42:5: error: conflicting types  
for 'coiltemp_program'  
/opt/topspin1.3/exp/stan/nmr/au/src/coiltemp:43:1: note: an argument type  
that has a default promotion can't match an empty parameter name list  
declaration  
/opt/topspin1.3/exp/stan/nmr/au/src/coiltemp:31:9: note: previous implicit  
declaration of 'coiltemp_program' was here  
exit 1  
/opt/topspin1.3/exp/stan/nmr/au/src/decra: In function 'AU_program':  
/opt/topspin1.3/exp/stan/nmr/au/src/decra:112:12: error: invalid storage  
class for function 'DECRA_program'  
/opt/topspin1.3/exp/stan/nmr/au/src/decra: At top level:  
/opt/topspin1.3/exp/stan/nmr/au/src/decra:293:12: error: static declaration  
of 'DECRA_program' follows non-static declaration  
/opt/topspin1.3/exp/stan/nmr/au/src/decra:115:9: note: previous implicit  
declaration of 'DECRA_program' was here  
exit 1  
/opt/topspin1.3/exp/stan/nmr/au/src/disconv: In function 'AU_program':  
/opt/topspin1.3/exp/stan/nmr/au/src/disconv:128:12: error: invalid storage  
class for function 'DISNMR_program'  
/opt/topspin1.3/exp/stan/nmr/au/src/disconv: At top level:  
/opt/topspin1.3/exp/stan/nmr/au/src/disconv:878:12: error: static  
declaration of 'DISNMR_program' follows non-static declaration  
/opt/topspin1.3/exp/stan/nmr/au/src/disconv:131:9: note: previous implicit  
declaration of 'DISNMR_program' was here  
exit 1  
/opt/topspin1.3/exp/stan/nmr/au/src/disinfo: In function 'AU_program':  
/opt/topspin1.3/exp/stan/nmr/au/src/disinfo:106:12: error: invalid storage  
class for function 'DISNMR_program'  
/opt/topspin1.3/exp/stan/nmr/au/src/disinfo: At top level:  
/opt/topspin1.3/exp/stan/nmr/au/src/disinfo:832:12: error: static  
declaration of 'DISNMR_program' follows non-static declaration  
/opt/topspin1.3/exp/stan/nmr/au/src/disinfo:109:9: note: previous implicit  
declaration of 'DISNMR_program' was here  
exit 1  
/opt/topspin1.3/exp/stan/nmr/au/src/lcsino:46:7: error: conflicting types
```

```
for 'lcsino'
/opt/topspin1.3/exp/stan/nmr/au/src/lcsino:40:7: note: previous implicit
declaration of 'lcsino' was here
exit 1
/opt/topspin1.3/exp/stan/nmr/au/src/multi_zgvd: In function 'AU_program':
/opt/topspin1.3/exp/stan/nmr/au/src/multi_zgvd:47:13: error: invalid storage
class for function 'PrintExpTime'
exit 1
/opt/topspin1.3/exp/stan/nmr/au/src/multi_zgvt: In function 'AU_program':
/opt/topspin1.3/exp/stan/nmr/au/src/multi_zgvt:54:13: error: invalid storage
class for function 'PrintExpTime'
exit 1
/opt/topspin1.3/exp/stan/nmr/au/src/multicmd: In function 'AU_program':
/opt/topspin1.3/exp/stan/nmr/au/src/multicmd:39:13: error: invalid storage
class for function 'PrintExpTime'
exit 1
/opt/topspin1.3/exp/stan/nmr/au/src/multiexpt: In function 'AU_program':
/opt/topspin1.3/exp/stan/nmr/au/src/multiexpt:29:13: error: invalid storage
class for function 'PrintExpTime'
exit 1
/opt/topspin1.3/exp/stan/nmr/au/src/multizg: In function 'AU_program':
/opt/topspin1.3/exp/stan/nmr/au/src/multizg:38:13: error: invalid storage
class for function 'PrintExpTime'
exit 1
/opt/topspin1.3/exp/stan/nmr/au/src/noemult: In function 'AU_program':
/opt/topspin1.3/exp/stan/nmr/au/src/noemult:53:13: error: invalid storage
class for function 'PrintExpTime'
exit 1
/opt/topspin1.3/exp/stan/nmr/au/src/pulsecalib: In function 'AU_program':
/opt/topspin1.3/exp/stan/nmr/au/src/pulsecalib:123:16: error: invalid
storage class for function 'pulsecalib'
/opt/topspin1.3/exp/stan/nmr/au/src/pulsecalib: At top level:
/opt/topspin1.3/exp/stan/nmr/au/src/pulsecalib:290:1: error: static
declaration of 'pulsecalib' follows non-static declaration
/opt/topspin1.3/exp/stan/nmr/au/src/pulsecalib:124:12: note: previous
implicit declaration of 'pulsecalib' was here
exit 1
/opt/topspin1.3/exp/stan/nmr/au/src/setproj:149:5: error: conflicting types
for 'sorter'
/opt/topspin1.3/exp/stan/nmr/au/src/setproj:35:5: note: previous declaration
of 'sorter' was here
exit 1
/opt/topspin1.3/exp/stan/nmr/au/src/simplex: In function 'AU_program':
/opt/topspin1.3/exp/stan/nmr/au/src/simplex:262:12: error: invalid storage
class for function 'SIMPLEX_program'
/opt/topspin1.3/exp/stan/nmr/au/src/simplex: At top level:
/opt/topspin1.3/exp/stan/nmr/au/src/simplex:468:12: error: static
declaration of 'SIMPLEX_program' follows non-static declaration
/opt/topspin1.3/exp/stan/nmr/au/src/simplex:265:9: note: previous implicit
declaration of 'SIMPLEX_program' was here
exit 1
```

<note important> Ara que els programes AU s'han compilat correctament, el problema és que quan els executo, tots donen el següent missatge d'error:

```
ILLEGAL TERMINATION of process 28469  
due to signal 11
```

potser pels motius explicats [aquí](#): *ldd with 32-bit binaries on 64-bit system - runs but won't report.*
</note>

From:
<https://sermn.uab.cat/wiki/> - **SeRMN Wiki**

Permanent link:
https://sermn.uab.cat/wiki/doku.php?id=informatica:hp_xw4300_500_topspin13_au_compilation&rev=1443526693

Last update: **2015/09/29 13:38**

