

Avance III 400 MHz SB - Altres tasques post-configuració del TopSpin

Aquesta pàgina conté les tasques posteriors a la instal·lació de les dues versions 3.6.3 i 3.6.4 del Topspin. Per exemple: organitzar les carpetes creades, eliminar les carpetes redundants o innecessàries, organitzar les carpetes de dades, etc.

Carpetes amb versions anteriors del TopSpin

- Mover les carpetes `/opt/topspin3.6.3/conf/instr/topspin3.5pl6` i `/opt/topspin3.6.3/conf/instr/topspin3.6.1` dins `/opt/topspin3.6.4/conf/instr`.
- Mover la carpeta `/opt/topspin3.6.3/` dins `/opt/topspin3.6.4/conf/instr`
- Eliminar de `/opt/topspin3.6.4/conf/instr/` les carpetes i fitxers innecessaris de les instal·lacions anteriors, entre altres: `examdata`, `guide`, `jython`, `prog/docu`, etc.

L'espai final ocupat pels fitxers de configuració de les anteriors instal·lacions és:

```
# du -hs topspin*
1.4G    topspin3.5pl6
1015M   topspin3.6.1
537M    topspin3.6.3
```

Discos durs HDD

Aquests són els discos durs HDD procedents d'altres ordinadors i instal·lats al nou ordinador.

Disc dur HDD de l'anterior ordinador del 400SB

- Model: WDC WD5003ABYZ-011FA0 (01.01S03)
 - Size: 500 GB (500,107,862,016 bytes)
 - Partitioning: MBR
 - Serial No: WD-WMAYP0J0AXNS
 - Mount point: `/dev/sdc`
 - Partitions:
 - `/dev/sdc1` - Ext2
 - `/dev/sdc2` - Extended Partition
 - `/dev/sdc5` - Linux LVM

amb la següent configuració de LVM,

```
# pvs /dev/sdc5
PV          VG          Fmt  Attr PSize   PFree
/dev/sdc5   cie-55-31-vg  lvm2  a--  <465.52g  5.98g
```

```
# vgs cie-55-31-vg
VG                #PV #LV #SN Attr   VSize   VFree
cie-55-31-vg      1   6   0 wz--n- <465.52g 5.98g

# lvs cie-55-31-vg
LV      VG                Attr          LSize   Pool Origin Data%  Meta%  Move Log
Cpy%Sync Convert
home    cie-55-31-vg -wi-ao---- 400.00g
opt      cie-55-31-vg -wi-ao---- 40.00g
root     cie-55-31-vg -wi-ao---- <8.38g
swap_1   cie-55-31-vg -wi-a----- <8.00g
tmp      cie-55-31-vg -wi-a----- 380.00m
var      cie-55-31-vg -wi-ao---- 2.79g
```



SMART indica que aquest disc ha estat en funcionament 4 anys i 3 mesos, però que no té cap problema. En qualsevol cas, **aquest disc dur no es farà servir al nou ordinador, i caldrà transferir el seu contingut al nou disc dur HDD.**

Disc dur HDD de l'anterior ordinador del 400WB

- Model: WDC WD10EZEX-60M2NA0 (03.01A03)
 - Size: 1.0 TB (1,000,204,886,016 bytes)
 - Partitioning: GUID Partition Table
 - Serial No: WD-WCC3F4CRTCZ4
 - Mount point: /dev/sdb
 - Partitions:
 - /dev/sdb1 - EFI System - Ext4 - 43 GB - ROOT
 - /dev/sdb2 - Linux Filesystem - Ext4 - 11 GB - VAR
 - /dev/sdb4 - Linux Filesystem - Ext4 - 21 GB - OPT
 - /dev/sdb5 - Linux Filesystem - Ext4 - 376 GB - HOME

SMART indica que aquest disc ha estat en funcionament 1 anys i 11 mesos, però que no té cap problema.

Després de comprovar que les dades de RMN ja es van transferir al servidor de dades, i de transferir algunes carpetes que podrien tenir un interès *històric*, esborro les particions al disc. Llavors creo dues particions de 500 GB cadascuna sense sistema de fitxers i començo a configurar-les per LVM,

```
# pvcreate /dev/sdb1 /dev/sdb2
Physical volume "/dev/sdb1" successfully created.
Physical volume "/dev/sdb2" successfully created.

# pvs /dev/sdb[1-9]
PV      VG                Fmt  Attr PSize   PFree
/dev/sdb1  cie-54-214-vg-2 lvm2 a-- 465.66g 465.66g
/dev/sdb2  cie-54-214-vg-2 lvm2 a-- <465.85g <465.85g
```

```
# vgcreate cie-54-214-vg-2 /dev/sdb1 /dev/sdb2
Volume group "cie-54-214-vg-2" successfully created

# vgs
VG                                #PV #LV #SN Attr   VSize   VFree
centos_cie-54-214                1   3   0 wz--n- <464.76g 4.00m
cie-54-214-vg-2                  2   0   0 wz--n- <931.51g <931.51g
cie-55-31-vg                     1   6   0 wz--n- <465.52g 5.98g

# lvcreate -L 200G -n current-data cie-54-214-vg-2
Logical volume "current-data" created.

# lvcreate -l 100%FREE -n archived-data cie-54-214-vg-2
Logical volume "archived-data" created.

# lvs cie-54-214-vg-2
LV          VG          Attr      LSize   Pool Origin Data%  Meta%
Move Log Cpy%Sync Convert
archived-data cie-54-214-vg-2 -wi-a----- <731.51g
current-data  cie-54-214-vg-2 -wi-a----- 200.00g

# lvdisplay cie-54-214-vg-2
--- Logical volume ---
LV Path                /dev/cie-54-214-vg-2/current-data
LV Name                 current-data
VG Name                 cie-54-214-vg-2
LV UUID                k1VFfK-f0hn-WPUS-ojPF-d89U-rzoj-MY1eWs
LV Write Access         read/write
LV Creation host, time cie-54-214.uab.cat, 2021-08-31 17:29:34 +0200
LV Status                available
# open                  0
LV Size                 200.00 GiB
Current LE              51200
Segments                1
Allocation              inherit
Read ahead sectors      auto
- currently set to      256
Block device            253:9
--- Logical volume ---
LV Path                /dev/cie-54-214-vg-2/archived-data
LV Name                 archived-data
VG Name                 cie-54-214-vg-2
LV UUID                RTFaLo-DXwm-xCNZ-5ELs-u8LM-4b8e-ahjZ4f
LV Write Access         read/write
LV Creation host, time cie-54-214.uab.cat, 2021-08-31 17:30:42 +0200
LV Status                available
# open                  0
LV Size                 <731.51 GiB
Current LE              187266
Segments                2
Allocation              inherit
```

Read ahead sectors	auto
- currently set to	256
Block device	253:10

i finalment creo el sistema de fitxers (ext4) a cadascun dels volums lògics,

```
# mkfs.ext4 /dev/mapper/cie--54--214--vg--2-current--data
mke2fs 1.42.9 (28-Dec-2013)
Filesystem label=
OS type: Linux
Block size=4096 (log=2)
Fragment size=4096 (log=2)
Stride=0 blocks, Stripe width=0 blocks
13107200 inodes, 52428800 blocks
2621440 blocks (5.00%) reserved for the super user
First data block=0
Maximum filesystem blocks=2199912448
1600 block groups
32768 blocks per group, 32768 fragments per group
8192 inodes per group
Superblock backups stored on blocks:
    32768, 98304, 163840, 229376, 294912, 819200, 884736, 1605632,
2654208,
    4096000, 7962624, 11239424, 20480000, 23887872
```

```
Allocating group tables: done
Writing inode tables: done
Creating journal (32768 blocks): done
Writing superblocks and filesystem accounting information: done
```

```
# mkfs.ext4 /dev/mapper/cie--54--214--vg--2-archived--data
mke2fs 1.42.9 (28-Dec-2013)
Filesystem label=
OS type: Linux
Block size=4096 (log=2)
Fragment size=4096 (log=2)
Stride=0 blocks, Stripe width=0 blocks
47947776 inodes, 191760384 blocks
9588019 blocks (5.00%) reserved for the super user
First data block=0
Maximum filesystem blocks=2340421632
5853 block groups
32768 blocks per group, 32768 fragments per group
8192 inodes per group
Superblock backups stored on blocks:
    32768, 98304, 163840, 229376, 294912, 819200, 884736, 1605632,
2654208,
    4096000, 7962624, 11239424, 20480000, 23887872, 71663616, 78675968,
102400000
```

```
Allocating group tables: done
Writing inode tables: done
Creating journal (32768 blocks): done
Writing superblocks and filesystem accounting information: done
```

Fitxer fstab

Creo les carpetes on es muntaran els nous sistemes de fitxers,

```
# mkdir -p nmrdata/current
# mkdir -p nmrdata/archive
# ls -l ../nmrdata/
total 8
drwxr-xr-x. 3 root root 4096 Aug 31 17:43 archive
drwxr-xr-x. 3 root root 4096 Aug 31 17:43 current
```

Afegeixo les següents línies al fitxer /etc/fstab per muntar els nous sistemes de fitxers,

```
## 20210831 - MCE - Espai de disc per dades actuals i antigues
##
/dev/mapper/cie--54--214--vg--2-current--data    /opt/nmrdata/current
ext4      defaults        0 0
/dev/mapper/cie--54--214--vg--2-archived--data  /opt/nmrdata/archive  ext4
defaults  0 0
```

i els munto

```
# mount -v /dev/mapper/cie--54--214--vg--2-current--data
mount: /opt/nmrdata/current does not contain SELinux labels.
       You just mounted an file system that supports labels which does not
       contain labels, onto an SELinux box. It is likely that confined
       applications will generate AVC messages and not be allowed access to
       this file system. For more details see restorecon(8) and mount(8).
mount: /dev/mapper/cie--54--214--vg--2-current--data mounted on
/opt/nmrdata/current.

# mount -v /dev/mapper/cie--54--214--vg--2-archived--data
mount: /opt/nmrdata/archive does not contain SELinux labels.
       You just mounted an file system that supports labels which does not
       contain labels, onto an SELinux box. It is likely that confined
       applications will generate AVC messages and not be allowed access to
       this file system. For more details see restorecon(8) and mount(8).
mount: /dev/mapper/cie--54--214--vg--2-archived--data mounted on
/opt/nmrdata/archive.
```



Resoldre el problema amb el SELinux

Enllaços d'interès

- [4.4.1. Creating Logical Volumes](#). Red Hat Documentation.
- ...

IN PROGRESS - Carpetes de dades



- Copiar les dades anteriors a la nova carpeta `"/opt/nmrdata/archive/"`.
- Moure les dades més recents a la nova carpeta `"/opt/nmrdata/current/"`.
- Agrupar els experiments dins archive segons la seva data. D'entrada, per anys, i més endavant per any i mes.

Còpia de les dades anteriors

Copio les dades de l'antic disc dur al nou disc dur,

```
# rsync -Hvax --progress --stats /mnt/old-400sb-home/sermnub/data/*
/opt/nmrdata/archive/
sending incremental file list
aaraujo/
aaraujo/nmr/
afinitica/
afinitica/nmr/
afinitica/nmr/AF-79-Saccharin_ACN/
afinitica/nmr/AF-79-Saccharin_ACN/1/
afinitica/nmr/AF-79-Saccharin_ACN/1/acqu
      8,834 100%    0.00kB/s    0:00:00 (xfr#1, ir-chk=1017/1387)
afinitica/nmr/AF-79-Saccharin_ACN/1/acqus
      9,006 100%    8.59MB/s    0:00:00 (xfr#2, ir-chk=1016/1387)
afinitica/nmr/AF-79-Saccharin_ACN/1/audita.txt
       701 100%   62.23kB/s    0:00:00 (xfr#3, ir-chk=1015/1387)
afinitica/nmr/AF-79-Saccharin_ACN/1/fid
:
:
test/nmr/tune-31P/1/pdata/1/thumb.png
      1,667 100%    3.73kB/s    0:00:00 (xfr#1159681, to-chk=2/1385013)
test/nmr/tune-31P/1/pdata/1/title
       13 100%    0.03kB/s    0:00:00 (xfr#1159682, to-chk=1/1385013)
venvirotech/
venvirotech/nmr/

Number of files: 1,385,013 (reg: 1,159,682, dir: 225,331)
Number of created files: 1,385,013 (reg: 1,159,682, dir: 225,331)
Number of deleted files: 0
```

```
Number of regular files transferred: 1,159,682
Total file size: 108,253,481,727 bytes
Total transferred file size: 108,253,481,727 bytes
Literal data: 108,253,481,727 bytes
Matched data: 0 bytes
File list size: 9,305,836
File list generation time: 0.001 seconds
File list transfer time: 0.000 seconds
Total bytes sent: 108,355,890,219
Total bytes received: 23,478,954

sent 108,355,890,219 bytes   received 23,478,954 bytes   33,179,050.72
bytes/sec
total size is 108,253,481,727   speedup is 1.00
```

Llavors moc les carpetes dels experiments de dins de les respectives carpetes nmr a la carpeta de cada grup, és a dir, de sermn/nmr a sermn,

```
# for DIR in *
> do
> mv $DIR/nmr/* $DIR
> done
mv: cannot stat 'aaraujo/nmr/*': No such file or directory
mv: cannot stat 'afinitica/nmr/*': No such file or directory
mv: cannot stat 'catechol/nmr/*': No such file or directory
mv: cannot stat 'esistare/nmr/*': No such file or directory
mv: cannot stat 'guest/nmr/*': No such file or directory
mv: cannot stat 'jaayllon/nmr/*': No such file or directory
mv: cannot stat 'lost+found/nmr/*': No such file or directory
mv: cannot stat 'nanomol/nmr/*': No such file or directory
mv: cannot stat 'nmarco/nmr/*': No such file or directory
mv: cannot stat 'venvirotech/nmr/*': No such file or directory
```

Per acabar, comprovo que no queda res dins les carpetes nmr abans d'esborrar-les,

```
# find ./*/nmr -type f -print
(finds nothing)

# du -hs ./*/nmr
4.0K    ./aaraujo/nmr
16K     ./afinitica/nmr
4.0K    ./afredi/nmr
4.0K    ./aponrouch/nmr
...
4.0K    ./sermn/nmr
4.0K    ./teo/nmr
4.0K    ./test/nmr
4.0K    ./venvirotech/nmr

# rm -ri ./*/nmr
rm: remove directory './aaraujo/nmr'? y
```

```
rm: remove directory './afinitica/nmr'? y
rm: remove directory './afredi/nmr'? y
...
rm: remove directory './sermn/nmr'? y
rm: remove directory './teo/nmr'? y
rm: remove directory './test/nmr'? y
rm: remove directory './venvirotech/nmr'? y
```

Carpets de dades actuals

Creo a /opt/nmrdata/current les mateixes carpets de dades que es varen crear als nous espectròmetres, per exemple, aquestes són les carpets creades a l'Avance Neo 400 MHz

```
[sermnadmin@sermn017 nmrdata]$ ls -w 80
afinitica      dmaspoch      iratera      lasem        ralibes      teo
aponrouch     druizmolina   jarbiol      lost+found   rokafuradada urquima
applus        dytquimica    jcasabo      miquel       rpleixats    venvirotech
avallribera   eva           jcbayon      miriam       sedq         vse
avirgili      fteixidor     jhernando    naliaga      sermn-data
cdomingo      gtobias       jpons        nanomol      sermn-test
cuantum       iberhospitex  jros         pau          synthesia
damabilino    interquim     jsuades      pq-qorg      teknokroma

[sermnadmin@sermn017 nmrdata]$ ls -l -I lost+found > folder-names.txt
```

Transfereixo el fitxer al nou ordinador de l'Avance III 400 MHz i creo les carpets de dades,

```
[root@cie-54-214 current] # for USER in `cat folder-names.txt`
> do
> mkdir --verbose $USER
> done
mkdir: created directory 'afinitica'
mkdir: created directory 'aponrouch'
mkdir: created directory 'applus'
mkdir: created directory 'avallribera'
[...]
mkdir: created directory 'urquima'
mkdir: created directory 'venvirotech'
mkdir: created directory 'vse'

# chown -R sermnuab:sermnuab [a-k,m-z]* lasem
[root@cie-54-214 current]# ls -l
total 192
drwxr-xr-x. 2 sermnuab sermnuab 4096 Sep  1 12:57 afinitica
drwxr-xr-x. 2 sermnuab sermnuab 4096 Sep  1 12:57 aponrouch
drwxr-xr-x. 2 sermnuab sermnuab 4096 Sep  1 12:57 applus
drwxr-xr-x. 2 sermnuab sermnuab 4096 Sep  1 12:57 avallribera
...
```

```
drwxr-xr-x. 2 sermnuab sermnuab 4096 Sep  1 12:57 jsuades
drwxr-xr-x. 2 sermnuab sermnuab 4096 Sep  1 12:57 lasem
drwx----- . 2 root      root      16384 Aug 31 17:43 lost+found
drwxr-xr-x. 2 sermnuab sermnuab 4096 Sep  1 12:57 miquel
...
drwxr-xr-x. 2 sermnuab sermnuab 4096 Sep  1 12:57 urquima
drwxr-xr-x. 2 sermnuab sermnuab 4096 Sep  1 12:57 venvirotech
drwxr-xr-x. 2 sermnuab sermnuab 4096 Sep  1 12:57 vse
```

Llavors, per cadascuna d'aquestes carpetes *actives*, moc les carpetes de dades més recents de archive a current. Ho faig a mà amb l'ajut del programa Mindight Commander després de [definir unes dreceres de teclat](#) per fer la tasca una mica menys feixuga.

- Quick search: **Ctrl+S**
- Sort by name: **Alt+#**
- Sort by MTime: **Alt+&**

IN PROGRESS - Compartir les carpetes de dades



- muntar la carpeta compartida al servidor de dades i muntar per separar current i archive.

Afegeixo les següents línies per compartir la carpeta de dades i la carpeta ~topspin/exp/stan/nmr/list amb el servidor de dades,

```
# SERMN - EXPORTED FOLDERS

# Export NMR data folder to SeRMN data server
# Because of SELinux, the data folder cannot be inside a home folder
/opt/nmrdata
sermn.uab.cat(ro,sync,no_subtree_check,root_squash,all_squash,insecure)

# Export TopSpin 3.6.4 lists folder to SeRMN data server
/opt/topspin3.6.4/exp/stan/nmr/lists
sermn.uab.cat(ro,sync,no_subtree_check,root_squash,all_squash,insecure)
```

i exporto les carpetes

```
# exportfs -v -a
exporting sermn.uab.cat:/opt/topspin3.6.4/exp/stan/nmr/lists
exporting sermn.uab.cat:/opt/nmrdata
exporting spect:/usr/diskless/clients/spect
exporting spect:/usr/diskless/dl_usr

# exportfs -v
/usr/diskless/dl_usr
spect(sync,wdelay,hide,no_subtree_check,sec=sys,ro,secure,root_squash,no_all_squash)
```

```
/usr/diskless/clients/spect
spect(sync,wdelay,hide,no_subtree_check,sec=sys,rw,secure,no_root_squash,no_
all_squash)
/opt/nmrdata
sermn.uab.cat(sync,wdelay,hide,no_subtree_check,sec=sys,ro,insecure,root_squ
ash,all_squash)
/opt/topspin3.6.4/exp/stan/nmr/lists
sermn.uab.cat(sync,wdelay,hide,no_subtree_check,sec=sys,ro,insecure,root_squ
ash,all_squash)
```

Configuració del TopSpin

Data Browser

Copio el fitxer browsedir2_Local.prop de l'Avance Neo 400 MHz dins la carpeta /home/sermnub/.topspin/prop i l'edito per canviar la ubicació de les carpetes de dades (/opt/nmrdata/current/) i eliminar els enllaços específics de l'altre espectròmetre. El resultat és,

```
$ cat browsedir2_Local.prop
#/home/sermnub/.topspin-cie-54-214/prop/browsedir2_Local.prop
#Wed Sep 01 17:35:11 CEST 2021
29=/opt/nmrdata/current/druizmolina\=alias\=D Ruiz-Molina - ICN2
28=/opt/nmrdata/current/dmaspoch\=alias\=D Maspoch - ICN2
27=/opt/nmrdata/current/pq-qorg\=alias\=Prac Quim Org
26=/opt/nmrdata/current/jhernando\=alias\=J Hernando - UAB
...
32=/opt/nmrdata/current/sermn-data\=alias\=SeRMN - NMR Data
31=/opt/nmrdata/current/rpleixats\=alias\=R Pleixats - UAB
30=/opt/nmrdata/current/ralibes\=alias\=R Alibes - UAB
```

Copio el fitxer a /home/sermnadmin/.topspin/prop perquè tots dos comptes vegin les mateixes carpetes.

Error setting parameter "LIFTMODE"



Cal consultar amb Bruker aquest error.

```
Error setting parameter "LIFTMODE": Parameter does not exist
(Original message = Error setting parameter "LIFTMODE": Parameter does not
exist)
```

```
=====
2 September 2021 10:47:14.947 +0200
```

```
Topspin Version = TopSpin 3.6.4 (of 2021-07-26 14:56:34), build 95
OS Name         = Linux 3.10.0-1160.25.1.el7.x86_64
JVM Version      = 1.8.0_242 (64 bit) AdoptOpenJDK
JVM Total memory = 170 MB
JVM Free  memory = 128 MB
```

```
java.lang.Exception: Stack trace
```

```
at
```

```
bruker.bio.topspin.bfw.gui.warn.AbstractMessage.getDetailsString(AbstractMessage.java:875)
```

```
at
```

```
bruker.bio.topspin.bfw.gui.warn.AbstractMessage.setMsgSource(AbstractMessage.java:837)
```

```
at
```

```
bruker.bio.topspin.bfw.gui.warn.AbstractMessage.<init>(AbstractMessage.java:821)
```

```
at de.bruker.nmr.mfw.base.BWarning.<init>(BWarning.java:59)
```

```
at de.bruker.nmr.mfw.base.BError.<init>(BError.java:50)
```

```
at de.bruker.nmr.sc.util.Misc.makeDialog(Misc.java:119)
```

```
at de.bruker.nmr.sc.util.Misc.showMsg(Misc.java:98)
```

```
at de.bruker.nmr.sc.util.Misc.showMsg(Misc.java:72)
```

```
at de.bruker.nmr.sc.util.Misc.showMsg(Misc.java:59)
```

```
at
```

```
de.bruker.nmr.sc.bsms.impl.BsmsCorbaUtil$1.run(BsmsCorbaUtil.java:147)
```

```
at java.lang.Thread.run(Thread.java:748)
```

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