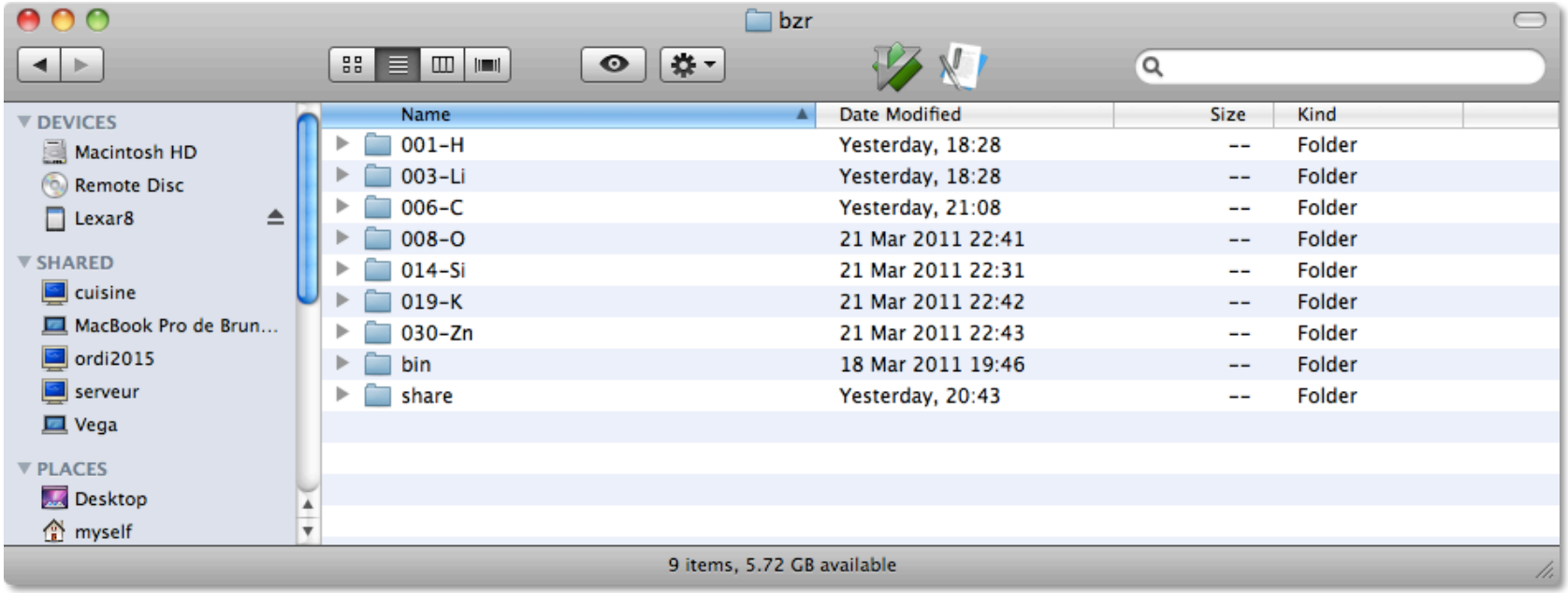
UCL
Université catholique de Louvain

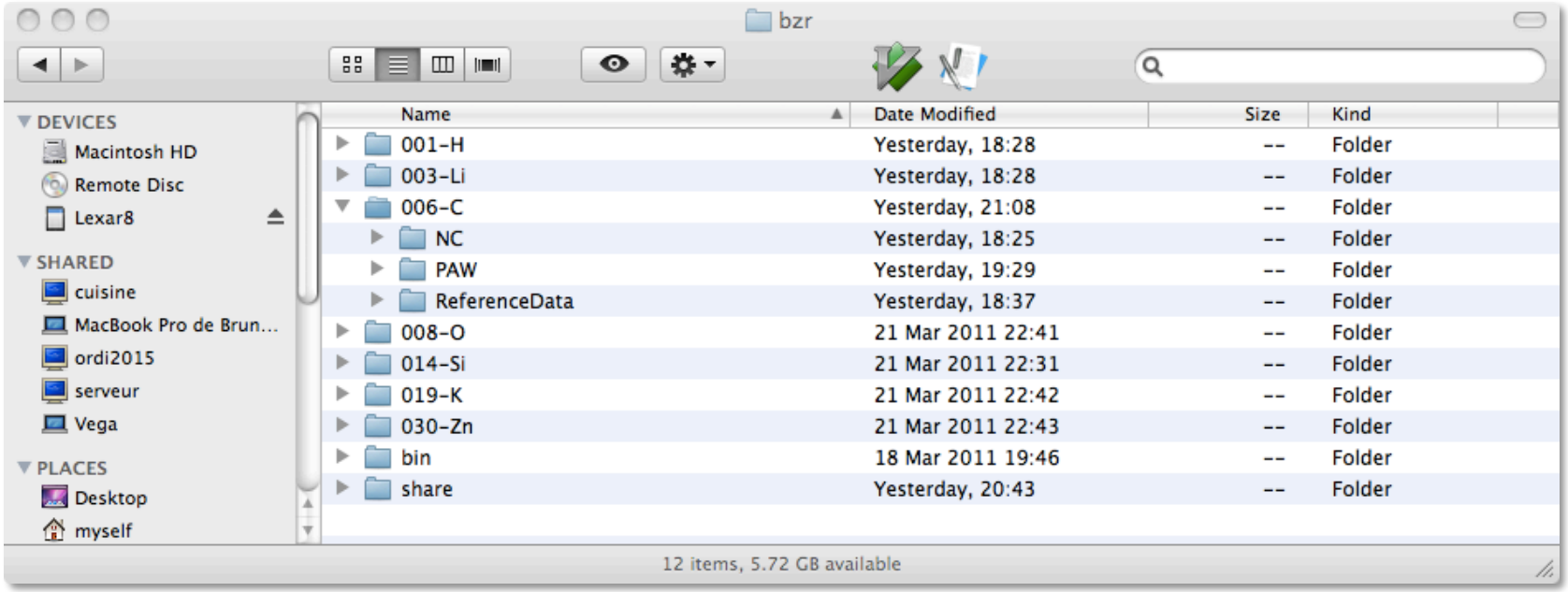
abinit/psps project

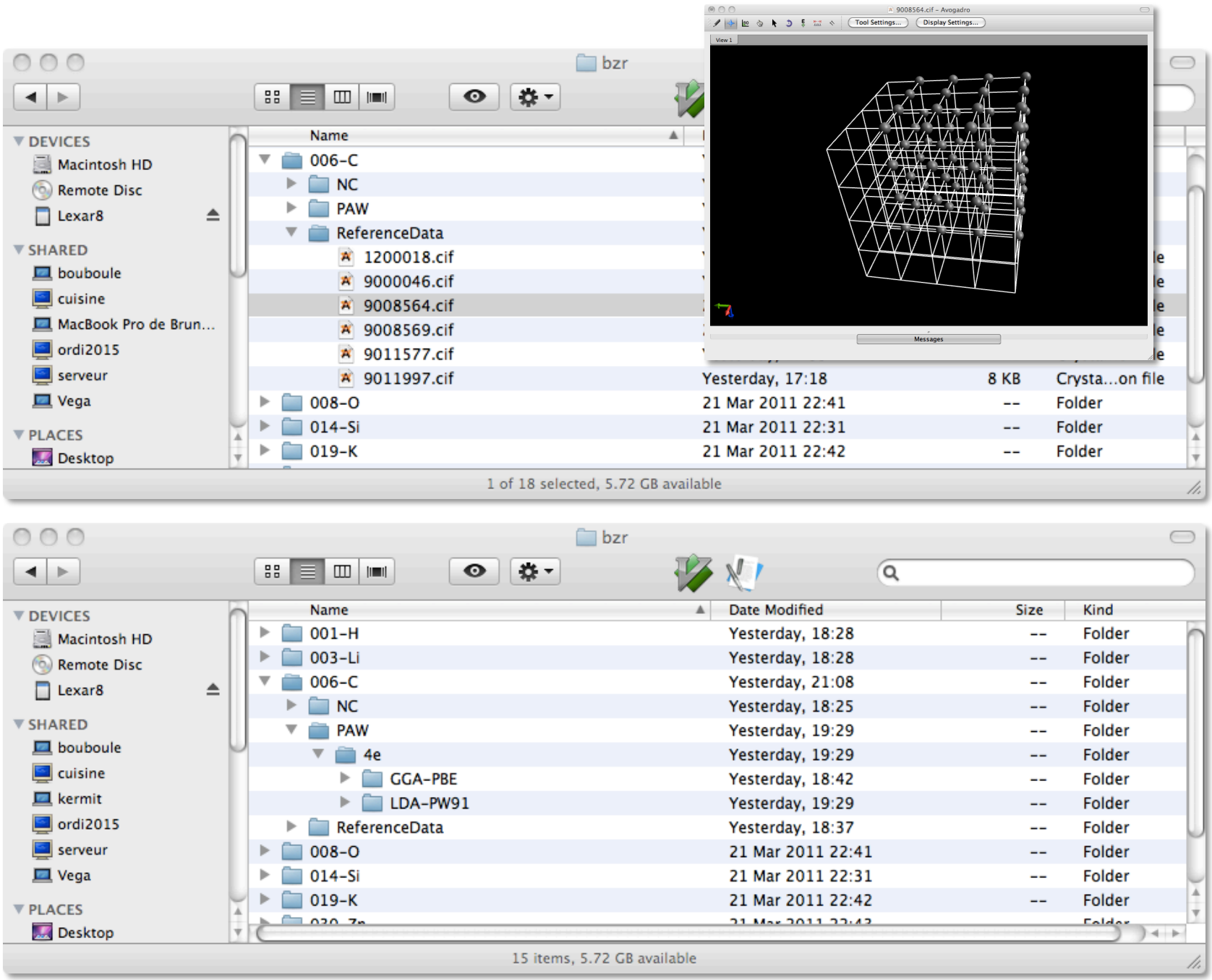
Access to the repositories … the usual location:

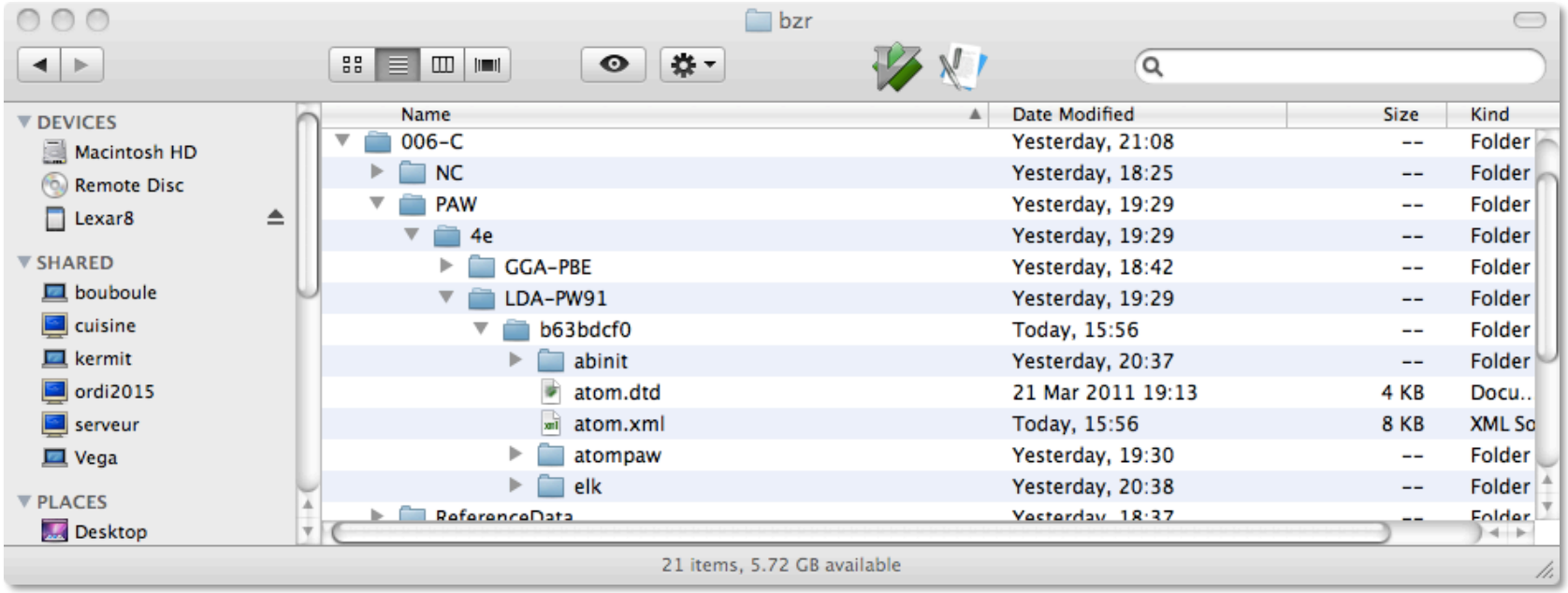
bzr+ssh://psps@archives.abinit.org/forge/psps/*xxx-AtomName*

xxx is 001-H to 112-Cn; one project per atom
repositories have one username – *psps* but use existing Abinit ssh keys


bzr
DEVICES
Macintosh HD
Remote Disc
Lexar8
SHARED
cuisine
MacBook Pro de Brun...
ordi2015
serveur
Vega
PLACES
Desktop
myself
Name
Date Modified
Size
Kind
001-H Yesterday, 18:28 -- Folder
003-Li Yesterday, 18:28 -- Folder
006-C Yesterday, 21:08 -- Folder
008-O 21 Mar 2011 22:41 -- Folder
014-Si 21 Mar 2011 22:31 -- Folder
019-K 21 Mar 2011 22:42 -- Folder
030-Zn 21 Mar 2011 22:43 -- Folder
bin 18 Mar 2011 19:46 -- Folder
share Yesterday, 20:43 -- Folder
9 items, 5.72 GB available


bzr
DEVICES
Macintosh HD
Remote Disc
Lexar8
SHARED
cuisine
MacBook Pro de Brun...
ordi2015
serveur
Vega
PLACES
Desktop
myself
Name
Date Modified
Size
Kind
001-H Yesterday, 18:28 -- Folder
003-Li Yesterday, 18:28 -- Folder
006-C Yesterday, 21:08 -- Folder
NC Yesterday, 18:25 -- Folder
PAW Yesterday, 19:29 -- Folder
ReferenceData Yesterday, 18:37 -- Folder
008-O 21 Mar 2011 22:41 -- Folder
014-Si 21 Mar 2011 22:31 -- Folder
019-K 21 Mar 2011 22:42 -- Folder
030-Zn 21 Mar 2011 22:43 -- Folder
bin 18 Mar 2011 19:46 -- Folder
share Yesterday, 20:43 -- Folder
12 items, 5.72 GB available


bzr
DEVICES
Macintosh HD
Remote Disc
Lexar8
SHARED
bouboule
cuisine
MacBook Pro de Brun...
ordi2015
serveur
Vega
PLACES
Desktop
Name
006-C
NC
PAW
ReferenceData
1200018.cif
9000046.cif
9008564.cif
9008569.cif
9011577.cif
9011997.cif
Yesterday, 17:18
8 KB
Crysta...on file
008-O
014-Si
019-K
21 Mar 2011 22:41
21 Mar 2011 22:31
21 Mar 2011 22:42
Folder
1 of 18 selected, 5.72 GB available
9008564.cif – Avogadro
Tool Settings...
Display Settings...
Messages
bzr
Date Modified
Size
Kind
001-H
003-Li
Yesterday, 18:28
Yesterday, 21:08
Yesterday, 18:25
Yesterday, 19:29
Yesterday, 18:42
Yesterday, 18:37
4e
GGA-PBE
LDA-PW91
ReferenceData
kermit
15 items, 5.72 GB available



UUID

Two-liner python code

```
>>> import uuid
>>> uuid.uuid1()
```

Conflicts between contributions

bzr merge before *bzr push*

atom.xml

```
<?xml version="1.0" encoding="UTF-8"?>
<atom version="1.0">
<dict>
        <key>DatasetName</key>
        <string>b63bdcf0-6391-11e0-b8af-5855caf38db7</string>
        <key>AtomicNumber</key>
        <integer>6</integer>
        <key>AtomName</key>
        <string>C</string>
…
        <key>XCFunctional</key>
        <dict>
              <key>ID</key>
              <integer>7</integer>
              <key>Name</key>
              <string>LDA-PW</string>
        </dict>
        <key>ScalarRelativistic</key>
        <true/>
        <key>GridSize</key>
        <integer>801</integer>
```

```
<key>CoreElectrons</key>
<integer>2</integer>
<key>ValenceElectrons</key>
<integer>4</integer>
<key>ElectronicConfiguration</key>
<dict>
        <key>1s</key>
        <dict>
                <key>State</key>
                <array>
                        <integer>1</integer>
                        <integer>0</integer>
                </array>
                <key>Occupation</key>
                <real>2.0</real>
                <key>Valence</key>
                <false/>
        </dict>
```

…

```
<key>PartialWaveBasis</key>
<dict>
        <key>MaximumLQuantumNumber</key>
        <integer>1</integer>
        <key>PartialWave</key>
        <dict>
                <key>State</key>
                <integer>0</integer>
                <key>ReferenceEnergy</key>
                <array>
                </array>
                <key>Unit</key>
                <string>Rydberg</string>
        </dict>
        <key>PartialWave</key>
        <dict>
                <key>State</key>
                <integer>1</integer>
                <key>ReferenceEnergy</key>
                <array>
                </array>
                <key>Unit</key>
                <string>Rydberg</string>
```

…

```
        <key>DataGenerator</key>
        <dict>
              <key>Name</key>
              <string>atompaw</string>
              <key>Version</key>
              <string>3.0.1</string>
        </dict>
        <key>DataConvertor</key>
        <dict>
              <key>Name</key>
              <string>AtomPAW2Abinit</string>
              <key>Version</key>
              <string></string>
        </dict>
…
        <key>DataValidator_2</key>
        <dict>
              <key>Name</key>
              <string>elk</string>
              <key>Version</key>
              <string>1.2.15</string>
        </dict>
```

```
        <key>Author</key>
        <dict>
                <key>Name</key>
                <string>Jacques Alain</string>
                <key>Address</key>
                <string>UCL PCPM</string>
                <key>Email</key>
                <string>alain.jacques@uclouvain.be</string>
        </dict>
</dict>
</atom>
```

Working directories

atompaw – abinit – elk

Naming conventions:

input files i.e. atompaw.in, abinit.in, elk.in

output files i.e. atompaw.log, abinit,log

Validation of the PAW pseudopotentials

follows guidelines of PAW3 tutorial, comparison between *Abinit* and an all -electron FP-LAPW code – *Elk*

on standardized systems: elemental solid, dimer, oxides, GS and GW

Open questions

- how to have a systematic approach on the whole table?
- robust submission engine – how to check for completeness?
- efficient validation routine – how to rebuild the database?