





The Unix Shell

Advanced Shell Tricks











"How should I do

this?"













Combine existing programs using pipes & filters

\$ wc -l *.pdb | sort | head -1











- Combine existing programs using pipes & filters
- Redirect output from programs to files

$$$$$
 wc -1 *.pdb > lengths









- Combine existing programs using pipes & filters
- Redirect output from programs to files
- Use variables to control program operation
- \$ SECRET_IDENTITY=Dracula
- \$ echo \$SECRET_IDENTITY

Dracula









- Combine existing programs using pipes & filters
- Redirect output from programs to files
- Use variables to control program operation

Very powerful when used together









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Very powerful when used together

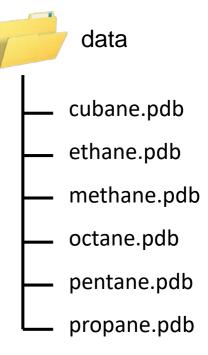
But there are other useful things we can do with these – let's take a look...













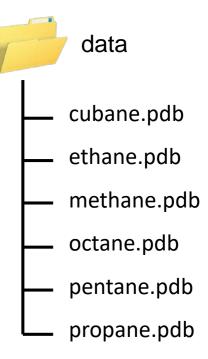








\$ ls *.pdb > files ← list all pdb files
 redirect to a file







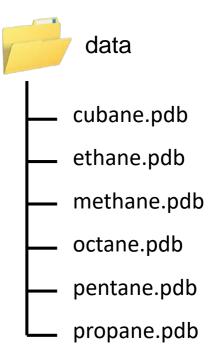






\$ 1s *.pdb > files — list all pdb files redirect to a file

The 'redirection' operator





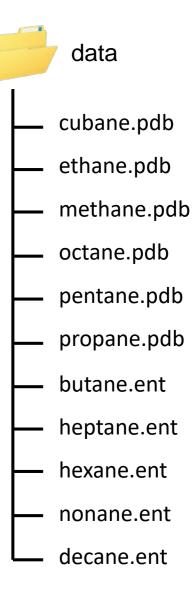








But what about adding this together with other results generated later?





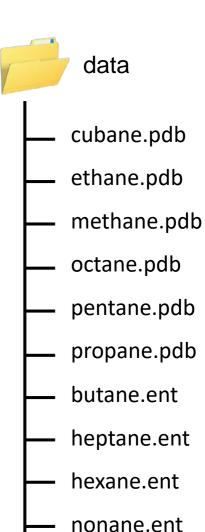








But what about adding this together with other results generated later?



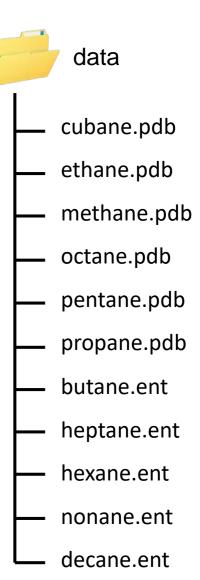








But what about adding this together with other results generated later?













But what about adding this together with other results generated later?

```
$ ls *.ent > more-files
```

\$ cat files more-files > all-files

append files into a single new file



data

cubane.pdb

ethane.pdb

methane.pdb

octane.pdb

pentane.pdb

propane.pdb

butane.ent

heptane.ent

hexane.ent

nonane.ent











But what about adding this together with other results generated later?

Instead, we can do...

append files into a single

\$ ls *.ent >> files new file



data

cubane.pdb

ethane.pdb

methane.pdb

octane.pdb

pentane.pdb

propane.pdb

butane.ent

heptane.ent

hexane.ent

nonane.ent











But what about adding this together with other results generated later?

append files

Instead, we can do...

Note the double >'s - the append' operator







data

cubane.pdb

ethane.pdb

methane.pdb

octane.pdb

pentane.pdb

propane.pdb

butane.ent

heptane.ent

hexane.ent

nonane.ent







We know that...

Normally, standard output is directed to a display:





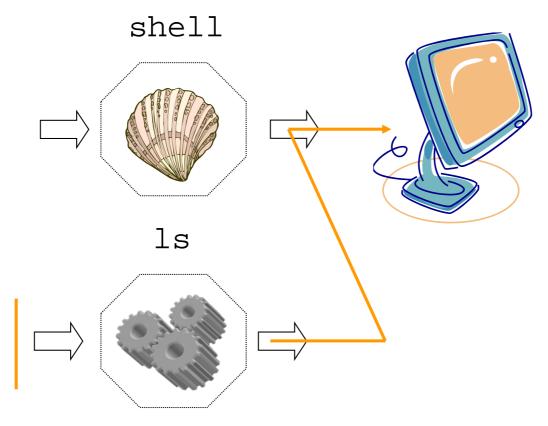






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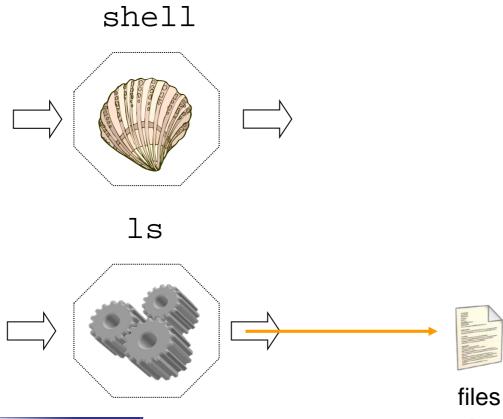




We know that...

Normally, standard output is directed to a display:

But we have redirected it to a file instead:























For example...

\$ ls /some/nonexistent/path > files
ls: /some/nonexistent/path: No such file or
directory









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directory

No files are listed in *files*, as you might expect.

But why isn't the error message in *files*?













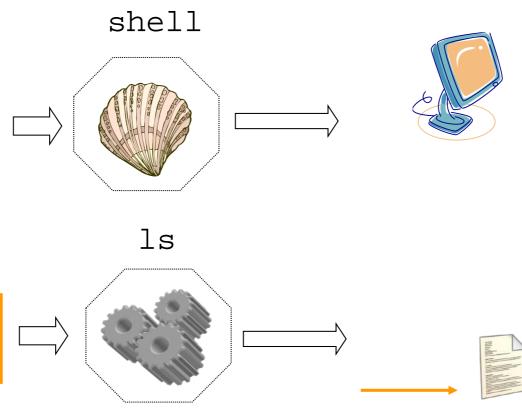






So what was happening with the previous

example?







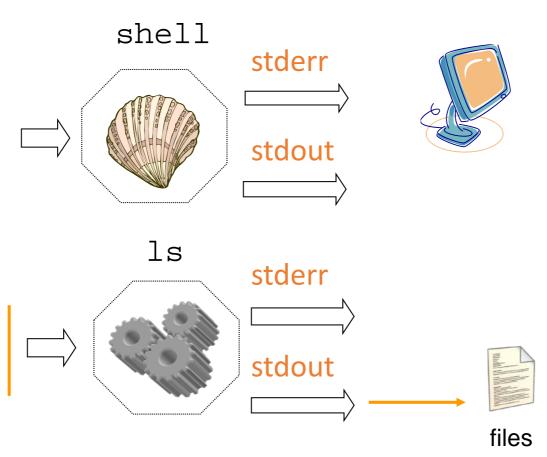






So what was happening with the previous

example?





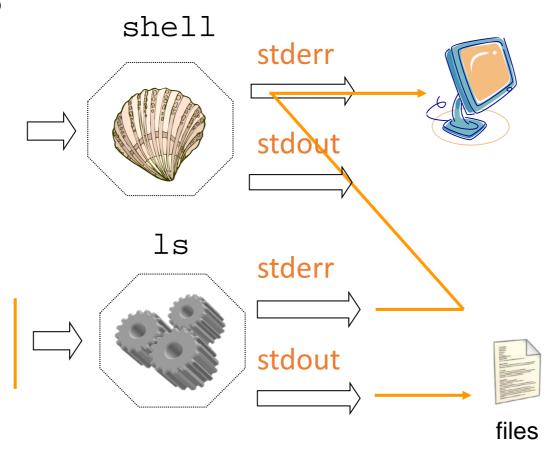






So what was happening with the previous

example?























To redirect the standard error to a file, we can do:

\$ ls /some/nonexistent/path 2> error-log

Redirect as before, but with a slightly different operator











To redirect the standard error to a file, we can do:

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Now we have any error messages stored in error-log







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To redirect both stdout and stderr, we can then do:

\$ ls /usr /some/nonexistent/path > files 2> error-log









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We can use both stdout and stderr redirection – at the same time











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To redirect both stdout and stderr, we can then do:

\$ ls /usr /some/nonexistent/path > files 2> error-log

Which would give us contents of /usr in files as well.











So why a '2' before the '>'?











So why a '2' before the '>'?

Both stdout and stderr can be referenced by numbers:

\$ ls /usr /some/nonexistent/path 1> files 2> error-log



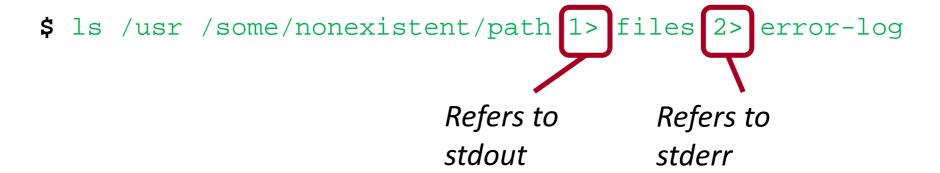






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Both stdout and stderr can be referenced by numbers:

\$ ls /usr /some/nonexistent/path 1> files 2> error-log

To just redirect both to the same file we can also do:

\$ ls /usr /some/nonexistent/path &> everything

With '&' denoting both stdout and stderr









So why a '2' before the '>'?

Both stdout and stderr can be referenced by numbers:

\$ ls /usr /some/nonexistent/path 1> files 2> error-log

To just redirect both to the same file we can also do:

\$ ls /usr /some/nonexistent/path &> everything

With '&' denoting both stdout and stderr

We can also use append for each of these too:

\$ ls /usr /some/nonexistent/path 1>> files 2>> error-log











>	1>	Redirect stdout to a file
	2>	Redirect stderr to a file
	&>	Redirect both stdout and stderr to the same file









>	1>	Redirect stdout to a file
	2>	Redirect stderr to a file
	&>	Redirect both stdout and stderr to the same file
>>	1>>	Redirect and append stdout to a file
	2>>	Redirect and append stderr to a file
	&>>	Redirect and append both stdout and stderr to a file











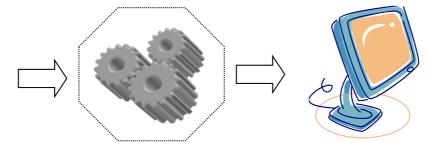








a_program 1 2 3













But what about running the same program separately, for each input?

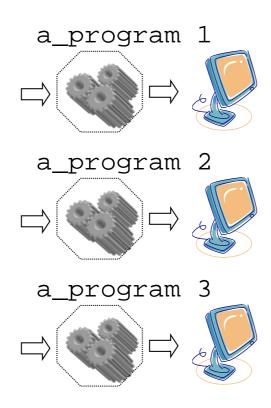








But what about running the same program separately, for each input?





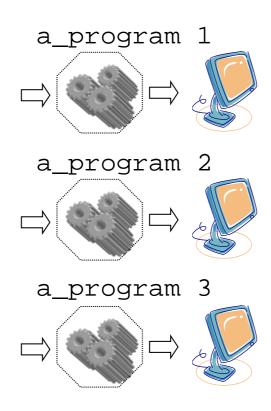








But what about running the same program separately, for each input?



We can use *loops* for this...













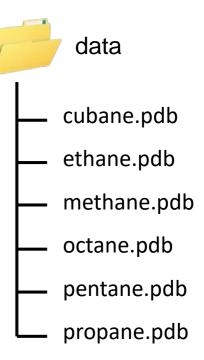








Let's go back to our first set of pdb files, and assume we want to compress each of them









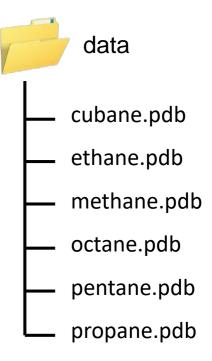




Let's go back to our first set of pdb files, and assume we want to compress each of them

We could do the following for each:

\$ zip cubane.pdb.zip cubane.pdb
adding: cubane.pdb (deflated 73%)









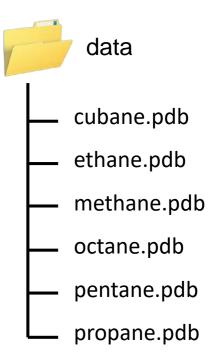




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typical output from the zip command











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We could do the following for each:

```
$ zip cubane.pdb.zip cubane.pdb
adding: cubane.pdb (deflated 73%)
```

The zip file we wish to create

typical output from the zip command

data

cubane.pdb

ethane.pdb

octane.pdb

pentane.pdb

propane.pdb

methane.pdb











Let's go back to our first set of pdb files, and assume we want to compress each of them

We could do the following for each:

\$ zip cubane.pdb.zip cubane.pdb
adding: cubane.pdb (deflated 73%)

The zip file we wish to create

The file(s)
we wish to
add to the
zip file

typical output from the zip command

data

cubane.pdb

ethane.pdb

octane.pdb

pentane.pdb

propane.pdb

methane.pdb











Let's go back to our first set of pdb files, and assume we want to compress each of them

We could do the following for each:



The zip file we wish to create

The file(s)
we wish to
add to the
zip file

typical output from the zip command

data

cubane.pdb

ethane.pdb

octane.pdb

pentane.pdb

propane.pdb

methane.pdb

Not efficient for many files











\$ for file in *.pdb; do zip \$file.zip \$file; done









```
for file in *.pdb; do zip $file.zip $file; done

For each pdb
file in this
directory...
```











```
$ for file in *.pdb; do zip $file.zip $file; done
```

Run this command











\$ for file in *.pdb; do zip \$file.zip \$file; done
This is the end
 of the loop











```
$ for file in *.pdb; do zip $file.zip $file; done
```

The semicolons separate each part of the loop construct











```
$ for file in *.pdb; do zip $file.zip $file; done
```

This expands to a list of every pdb file









```
$ for file in *.pdb; do zip $file.zip $file; done
```

This variable holds the next pdb file in the list









```
$ for file in *.pdb; do zip $file.zip $file; done
```

We reference the 'file' variable, and use '.' to add the zip extension to the filename









\$ for file in *.pdb; do zip \$file.zip \$file; done

We reference the

'file' variable again











```
$ for file in *.pdb; do zip $file.zip $file; done
adding: cubane.pdb (deflated 73%)
adding: ethane.pdb (deflated 70%)
adding: methane.pdb (deflated 66%)
adding: octane.pdb (deflated 75%)
adding: pentane.pdb (deflated 74%)
adding: propane.pdb (deflated 71%)
```









```
$ for file in *.pdb; do zip $file.zip $file; done
adding: cubane.pdb (deflated 73%)
adding: ethane.pdb (deflated 70%)
...
```

In one line, we've ended up with all files zipped









```
$ for file in *.pdb; do zip $file.zip $file; done
adding: cubane.pdb (deflated 73%)
adding: ethane.pdb (deflated 70%)
...
```

In one line, we've ended up with all files zipped

```
$ ls *.zip
cubane.pdb.zip methane.pdb.zippentane.pdb.zip
ethane.pdb.zip octane.pdb.zip propane.pdb.zip
```

















We could use head -1 *.pdb for that, but it would produce:

```
==> cubane.pdb <==
COMPND CUBANE

==> ethane.pdb <==
COMPND ETHANE

==> methane.pdb <==
COMPND METHANE</pre>
```









We could use head -1 *.pdb for that, but it would produce:

head produces this

==> cubane.pdb <== (it's not in the file)

CUBANE

==> ethane.pdb <== COMPND ETHANE

==> methane.pdb <== COMPND METHANE

•••

COMPND









We could use head -1 *.pdb for that, but it would produce:

head produces this

==> cubane.pdb <== ← (it's not in the file)

COMPND CUBANE ← this is actually the first line in this file!

==> ethane.pdb <== COMPND ETHANE

==> methane.pdb <== COMPND METHANE

•••









We could use head -1 *.pdb for that, but it would produce:

```
==> cubane.pdb <==
COMPND CUBANE

==> ethane.pdb <==
COMPND ETHANE

==> methane.pdb <==
COMPND METHANE
```

Perhaps we only want the actual first lines...











However, using a loop:











However, using a loop:

\$ for file in *.pdb; do head -1 \$file; done









However, using a loop:

```
$ for file in *.pdb; do head -1 $file; done
```

We use \$file as we did before, but this time with the head command











However, using a loop:

\$ for file in *.pdb; do head -1 \$file; done

COMPND CUBANE

COMPND ETHANE

COMPND METHANE

COMPND OCTANE

COMPND PENTANE

COMPND PROPANE



















Simple!

```
$ (for file in ls *.pdb; do head -1 $file; done) | sort -r
```











Simple!

```
$ (for file in ls *.pdb; do head -1 $file; done) sort -r
```

Using a pipe, we can just add this on the end











Simple!









zip	Create a compressed zip file with other files in it
for; do done;	Loop over a list of data and run a command once for each element in the list









created by

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July 2011



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All this typing is giving me RSI

 Didn't we use a file to store the commands in earlier examples?







All this typing is giving me RSI

 Didn't we use a file to store the commands in earlier examples?

Yes we did. Let's have a look at how that works...







• If you put commands in a file and chmod the file to be executable then you can run the file as a command.

```
$ cat > y.sh
for i in *
do
echo == $i ==
head -1 $i
tail -1 $i
Done
$ chmod 700 y.sh
```













What happens when I try to run a file that is not a script?

```
$ more a.txt
Hi there
this
is
file a
Xxx
```







Unintended consequences

```
$ chmod 700 a.txt
$ ./a.txt: line 1: Hi: command not found
./a.txt: line 2: this: command not found
./a.txt: line 3: is: command not found
a: cannot open 'a' (No such file or
directory)
./a.txt: line 5: xxx: command not found
$
```

Hi there
this
is
file a







How to make sure your script is a script

- 1) Only use the execute (x) permission if you are going to execute it.
- 2) Use an interpreter header as the first line of the file. (You can use the which bash to find your bash programs location.)

```
#!/bin/bash
for j in *
```







What about other control structures

- if test -e myfile; then ...; fi
- case ...; esac
- while ...
- I'm not going to tell you because
- 1) You can find this out on your own (man bash)
- 2) If you find yourself using if and case then you should probably switch to a programming language like python. It's safer.





