

# Practical Computing for Scientists

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UOIT – Fall 2015

# Assignment 1



- Please complete and submit Assignment 1:
  - Blackboard > Course Content > Week 3 (Sept. 28-Oct. 2) > Monday Sept. 28 > Assignment 1
  - Due Oct. 3, 2015, 17:00 EDT



# The Unix Shell

## Variables

Created by Greg Wilson

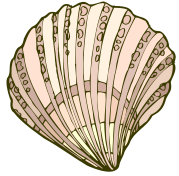


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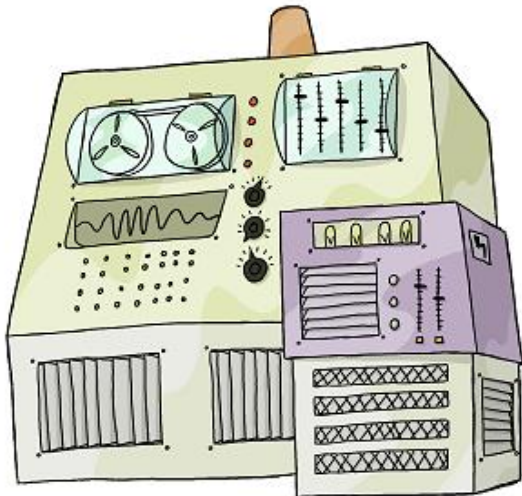
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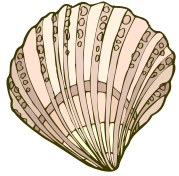
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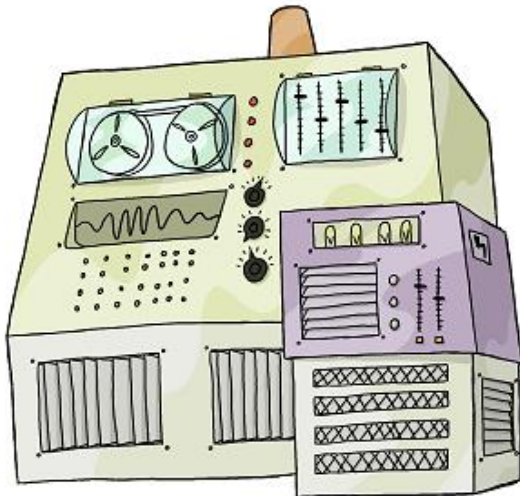
shell

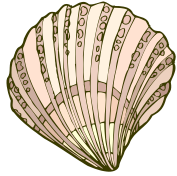




shell

The shell is a program

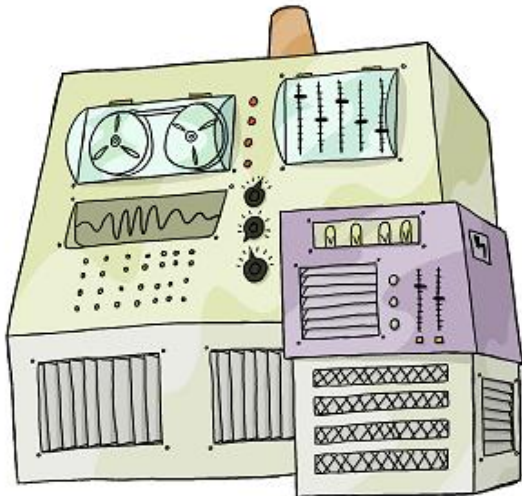


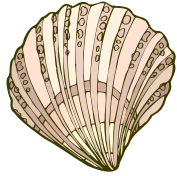


shell

The shell is a program

It has variables





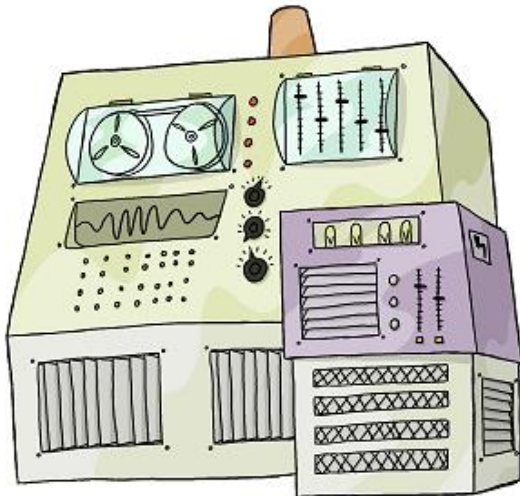
shell

The shell is a program

It has variables

Changing their values

changes its behavior



```
$ set
```

```
COMPUTERNAME=TURING
```

```
HOME=/home/vlad
```

```
HOMEDRIVE=C:
```

```
HOSTNAME=TURING
```

```
HOSTTYPE=i686
```

```
MANPATH=/usr/local/man:/usr/share/man:/usr/man
```

```
NUMBER_OF_PROCESSORS=4
```

```
OS=Windows_NT
```

```
PATH=/usr/local/bin:/usr/bin:/bin:/cygdrive/c/Windows/system32:
```

```
/cygdrive/c/Windows:/cygdrive/c/bin:/cygdrive/c/Python27
```

```
PWD=/home/vlad
```

```
UID=1000
```

```
USERNAME=vlad
```



\$ **set**



With no arguments, shows all variables and their values

COMPUTERNAME=TURING

HOME=/home/vlad

HOMEDRIVE=C:

HOSTNAME=TURING

HOSTTYPE=i686

MANPATH=/usr/local/man:/usr/share/man:/usr/man

NUMBER\_OF\_PROCESSORS=4

OS=Windows\_NT

PATH=/usr/local/bin:/usr/bin:/bin:/cygdrive/c/Windows/system32:

/cygdrive/c/Windows:/cygdrive/c/bin:/cygdrive/c/Python27

PWD=/home/vlad

UID=1000

USERNAME=vlad

```
$ set
```

```
COMPUTERNAME=TURING
```

Standard to use upper-case names

```
HOME=/home/vlad
```

```
HOMEDRIVE=C:
```

```
HOSTNAME=TURING
```

```
HOSTTYPE=i686
```

```
MANPATH=/usr/local/man:/usr/share/man:/usr/man
```

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NUMBER_OF_PROCESSORS=4
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PATH=/usr/local/bin:/usr/bin:/bin:/cygdrive/c/Windows/system32:
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```

```
PWD=/home/vlad
```

```
UID=1000
```

```
USERNAME=vlad
```

```
$ set
```

```
COMPUTERNAME=TURING
```

← All values are strings

```
HOME=/home/vlad
```

```
HOMEDRIVE=C:
```

```
HOSTNAME=TURING
```

```
HOSTTYPE=i686
```

```
MANPATH=/usr/local/man:/usr/share/man:/usr/man
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$ set
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PATH=/usr/local/bin:/usr/bin:/bin:/cygdrive/c/Windows/system32:
```

```
/cygdrive/c/Windows:/cygdrive/c/bin:/cygdrive/c/Python27
```

```
PWD=/home/vlad
```

```
UID=1000
```

```
USERNAME=vlad
```

← All values are strings

Programs must convert to other types when/as necessary

```
$ set
```

```
COMPUTERNAME=TURING
```

```
HOME=/home/vlad
```

```
HOMEDRIVE=C:
```

```
HOSTNAME=TURING
```

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PATH=/usr/local/bin:/usr/bin:/bin:/cygdrive/c/Windows/system32:
```

```
/cygdrive/c/Windows:/cygdrive/c/bin:/cygdrive/c/Python27
```

```
PWD=/home/vlad
```

```
UID=1000
```

```
USERNAME=vlad
```

`int(string)` for numbers



```
$ set
```

```
COMPUTERNAME=TURING
```

```
HOME=/home/vlad
```

```
HOMEDRIVE=C:
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PATH=/usr/local/bin:/usr/bin:/bin:/cygdrive/c/Windows/system32  
/cygdrive/c/Windows:/cygdrive/c/bin:/cygdrive/c/Python27
```

```
PWD=/home/vlad
```

```
UID=1000
```

```
USERNAME=vlad
```

split(':') for lists



`PATH` controls where the shell looks for programs

PATH controls where the shell looks for programs

\$ ./analyze ← Run the analyze program  
in the current directory



PATH controls where the shell looks for programs

```
$ ./analyze
```

```
$ /bin/analyze
```

← Run the `analyze` program  
in the `/bin` directory

PATH controls where the shell looks for programs

```
$ ./analyze
```

```
$ /bin/analyze
```

```
$ analyze
```

PATH controls where the shell looks for programs

```
$ ./analyze
```

```
$ /bin/analyze
```

```
$ analyze
```



```
directories = split(PATH, ':')
```

```
for each directory:
```

```
    if directory/analyze exists, run it
```

PATH controls where the shell looks for programs

```
$ ./analyze
```

```
$ /bin/analyze
```

```
$ analyze
```

```
/usr/local/bin
```

```
/usr/bin
```

```
/bin
```

```
/cygdrive/c/Windows/system32
```

```
/cygdrive/c/Windows
```

```
/cygdrive/c/bin
```

```
/cygdrive/c/Python27
```

PATH controls where the shell looks for programs

```
$ ./analyze
```

```
$ /bin/analyze
```

```
$ analyze
```

```
/usr/local/bin
```

```
/usr/bin
```

```
/bin
```

```
/cygdrive/c/Windows/system32
```

```
/cygdrive/c/Windows
```

```
/cygdrive/c/bin
```

```
/cygdrive/c/Python27
```

```
/bin/analyze
```

```
/cygdrive/c/bin/analyze
```

```
/users/vlad/analyze
```

PATH controls where the shell looks for programs

```
$ ./analyze  
$ /bin/analyze  
$ analyze
```

```
/usr/local/bin  
/usr/bin  
/bin  
/cygdrive/c/Windows/system32  
/cygdrive/c/Windows  
/cygdrive/c/bin  
/cygdrive/c/Python27
```

`/bin/analyze`

`/cygdrive/c/bin/analyze`

`/users/vlad/analyze`

PATH controls where the shell looks for programs

```
$ ./analyze
```

```
$ /bin/analyze
```

```
$ analyze
```

```
/usr/local/bin
```

```
/usr/bin
```

```
/bin
```

```
/cygdrive/c/Windows/system32
```

```
/cygdrive/c/Windows
```

```
/cygdrive/c/bin
```

```
/cygdrive/c/Python27
```

```
/bin/analyze
```

```
/cygdrive/c/bin/analyze
```

```
/users/vlad/analyze
```

echo prints its arguments



echo prints its arguments

Use it to show variables' values

echo prints its arguments

Use it to show variables' values

```
$ echo hello transylvania!
```

```
hello transylvania!
```

```
$
```

echo prints its arguments

Use it to show variables' values

```
$ echo hello transylvania!
```

```
hello transylvania!
```

```
$ echo HOME
```

echo prints its arguments

Use it to show variables' values

```
$ echo hello transylvania!
```

```
hello transylvania!
```

```
$ echo HOME
```

```
HOME
```

```
$
```

echo prints its arguments

Use it to show variables' values

```
$ echo hello transylvania!
```

```
hello transylvania!
```

```
$ echo HOME
```

```
HOME
```

```
$ echo $HOME
```

```
/home/vlad
```

```
$
```

echo prints its arguments

Use it to show variables' values

```
$ echo hello transylvania!
```

```
hello transylvania!
```

```
$ echo HOME
```

```
HOME
```

```
$ echo $HOME
```

```
/home/vlad
```

```
$
```

Ask shell to replace variable name  
with value before program runs



echo prints its arguments

Use it to show variables' values

```
$ echo hello transylvania!
```

```
hello transylvania!
```

```
$ echo HOME
```

```
HOME
```

```
$ echo $HOME
```

```
/home/vlad
```

```
$
```

Ask shell to replace variable name  
with value before program runs  
Just like \* and ? are expanded  
before the program runs

echo prints its arguments

Use it to show variables' values

```
$ echo hello transylvania!
```

```
hello transylvania!
```

```
$ echo HOME
```

```
HOME
```

```
$ echo $HOME → echo /home/vlad
```

```
/home/vlad
```

```
$
```



Create variable by assigning to it

Create variable by assigning to it

Change values by reassigning to existing variables

Create variable by assigning to it

Change values by reassigning to existing variables

```
$ SECRET_IDENTITY=Dracula
```

```
$ echo $SECRET_IDENTITY
```

```
Dracula
```

```
$ SECRET_IDENTITY=Camilla
```

```
$ echo $SECRET_IDENTITY
```

```
Camilla
```

```
$
```

Assignment only changes variable's value  
in *this* shell

Assignment only changes variable's value  
in *this* shell

```
$ SECRET_IDENTITY=Dracula
```

```
$ echo $SECRET_IDENTITY
```

```
Dracula
```

```
$
```

Assignment only changes variable's value  
in *this* shell

```
$ SECRET_IDENTITY=Dracula
```

```
$ echo $SECRET_IDENTITY
```

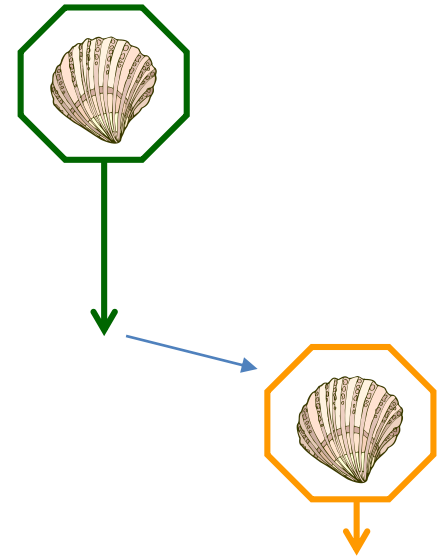
```
Dracula
```

```
$ bash
```

```
$
```

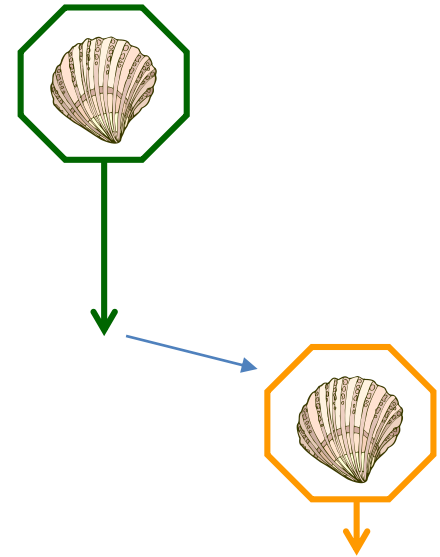
Assignment only changes variable's value  
in *this* shell

```
$ SECRET_IDENTITY=Dracula  
$ echo $SECRET_IDENTITY  
Dracula  
$ bash  
$
```



Assignment only changes variable's value  
in *this* shell

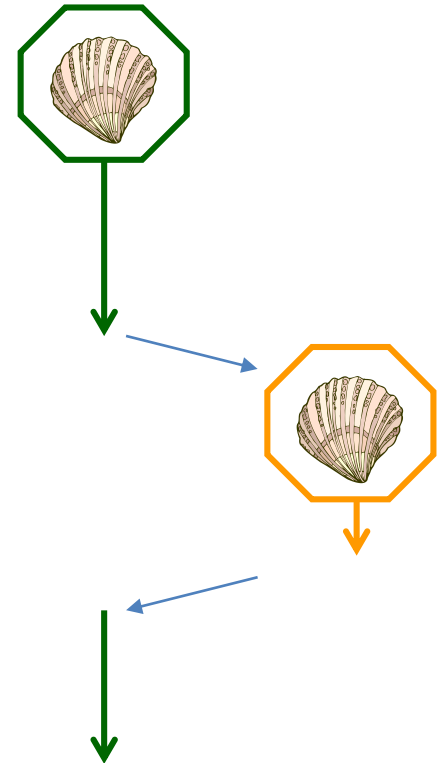
```
$ SECRET_IDENTITY=Dracula
$ echo $SECRET_IDENTITY
Dracula
$ bash
$ echo $SECRET_IDENTITY
$
```





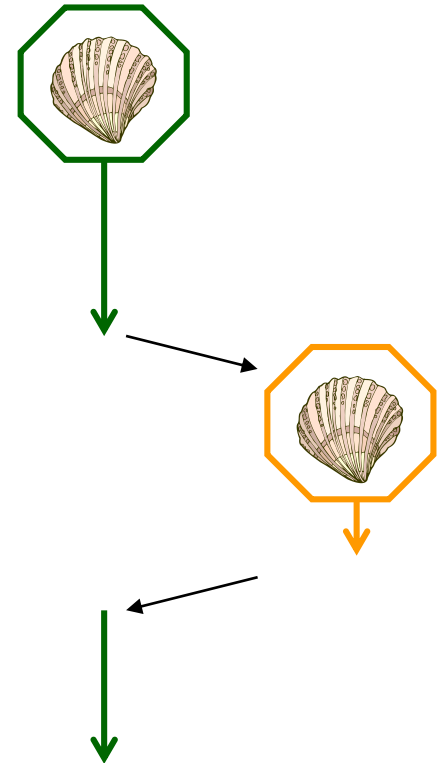
Assignment only changes variable's value  
in *this* shell

```
$ SECRET_IDENTITY=Dracula
$ echo $SECRET_IDENTITY
Dracula
$ bash
$ echo $SECRET_IDENTITY
$ exit
$
```



Assignment only changes variable's value  
in *this* shell

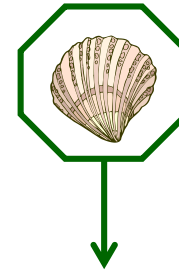
```
$ SECRET_IDENTITY=Dracula
$ echo $SECRET_IDENTITY
Dracula
$ bash
$ echo $SECRET_IDENTITY
$ exit
$ echo $SECRET_IDENTITY
Dracula
$
```



Use `export` to signal that the variable should be visible to subprocesses

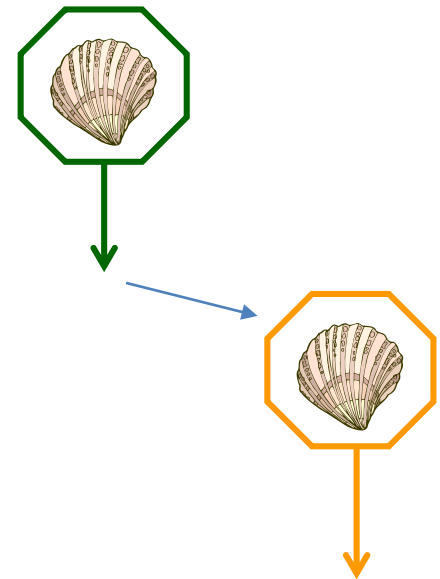
Use `export` to signal that the variable should be visible to subprocesses

```
$ SECRET_IDENTITY=Dracula  
$ export SECRET_IDENTITY  
$
```



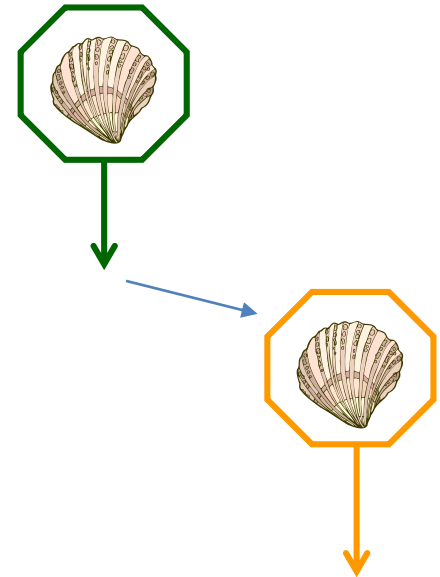
Use `export` to signal that the variable should be visible to subprocesses

```
$ SECRET_IDENTITY=Dracula  
$ export SECRET_IDENTITY  
$ bash  
$
```



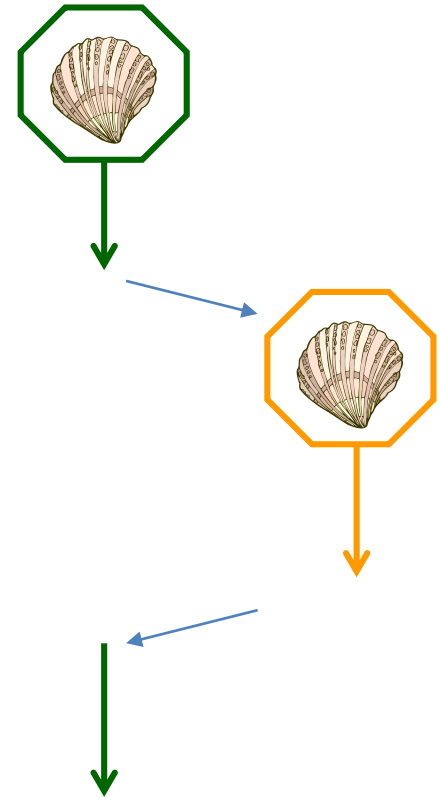
Use `export` to signal that the variable should be visible to subprocesses

```
$ SECRET_IDENTITY=Dracula
$ export SECRET_IDENTITY
$ bash
$ echo $SECRET_IDENTITY
Dracula
$
```



Use `export` to signal that the variable should be visible to subprocesses

```
$ SECRET_IDENTITY=Dracula
$ export SECRET_IDENTITY
$ bash
$ echo $SECRET_IDENTITY
Dracula
$ exit
$
```



Commands in `$HOME/.bashrc` are executed  
when shell starts



Commands in `$HOME/.bashrc` are executed  
when shell starts

```
export SECRET_IDENTITY=Dracula  
export BACKUP_DIR=$HOME/backup
```

```
/home/vlad/.bashrc
```

Commands in `$HOME/.bashrc` are executed  
when shell starts

```
export SECRET_IDENTITY=Dracula  
export BACKUP_DIR=$HOME/backup
```

Also common to use `alias` to create shortcuts

Commands in `$HOME/.bashrc` are executed when shell starts

```
export SECRET_IDENTITY=Dracula  
export BACKUP_DIR=$HOME/backup
```

Also common to use `alias` to create shortcuts

```
alias backup=/bin/zarble -v --nostir -R 20000 $HOME $BACKUP_DIR
```

Commands in `$HOME/.bashrc` are executed  
when shell starts

```
export SECRET_IDENTITY=Dracula  
export BACKUP_DIR=$HOME/backup
```

Also common to use `alias` to create shortcuts

```
alias backup=/bin/zarble -v --nostir -R 20000 $HOME $BACKUP_DIR
```

Not something you want to type over and over

# The Unix Shell

## Advanced Shell Tricks

Created by Steve Crouch



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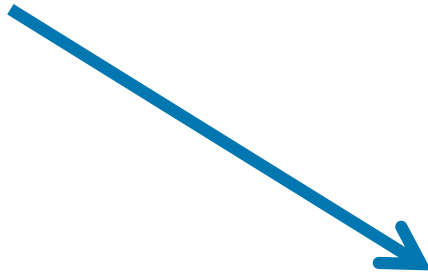
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"How should I do  
this?"



Some  
technical  
problem...



"How should I do this?"

With smartphones, you'll often hear people say something like

*"There's an app for that... check this out!"*





"How should I do this?"

With smartphones, you'll often hear people say something like

*"There's an app for that... check this out!"*



Whereas Unix shell programmers will say

*"There's a shell trick for that... check this out!"*



In previous lessons, we've seen how to:

- Combine existing programs using pipes & filters

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

In previous lessons, we've seen how to:

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

```
$ wc -l *.pdb > lengths
```

In previous lessons, we've seen how to:

- 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
```

In previous lessons, we've seen how to:

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

Very powerful when used together

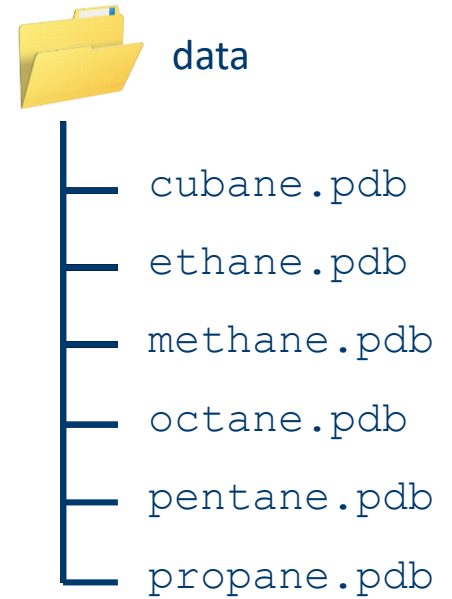
In previous lessons, we've seen how to:

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

Very powerful when used together

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

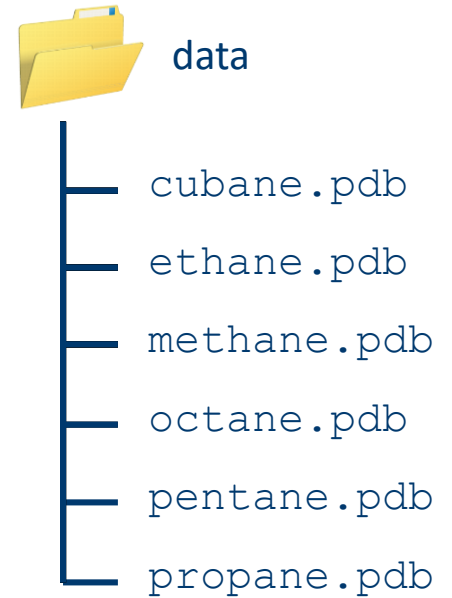
First, let's revisit redirection...



First, let's revisit redirection...

```
$ ls *.pdb > files
```

← list all pdb files  
redirect to a file

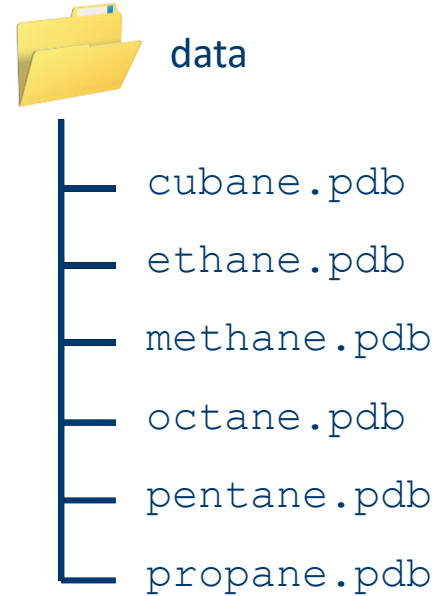


First, let's revisit redirection...

```
$ ls *.pdb > files
```

list all pdb files  
redirect to a file

The 'redirection'  
operator





First, let's revisit redirection...

```
$ ls *.pdb > files
```

← list all pdb files  
redirect to a file

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



data

- cubane.pdb
- ethane.pdb
- methane.pdb
- octane.pdb
- pentane.pdb
- propane.pdb
- butane.ent
- heptane.ent
- hexane.ent
- nonane.ent
- decane.ent

First, let's revisit redirection...

```
$ ls *.pdb > files
```

← list all pdb files  
redirect to a file

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

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



data

- cubane.pdb
- ethane.pdb
- methane.pdb
- octane.pdb
- pentane.pdb
- propane.pdb
- butane.ent
- heptane.ent
- hexane.ent
- nonane.ent
- decane.ent

First, let's revisit redirection...

```
$ ls *.pdb > files
```

← list all pdb files  
redirect to a file

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

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

We just want  
the ent files



data

- cubane.pdb
- ethane.pdb
- methane.pdb
- octane.pdb
- pentane.pdb
- propane.pdb
- butane.ent
- heptane.ent
- hexane.ent
- nonane.ent
- decane.ent

First, let's revisit redirection...

```
$ ls *.pdb > files
```

← list all pdb files  
redirect to a file

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
- decane.ent

First, let's revisit redirection...

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

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

Instead, we can do...

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



data

- cubane.pdb
- ethane.pdb
- methane.pdb
- octane.pdb
- pentane.pdb
- propane.pdb
- butane.ent
- heptane.ent
- hexane.ent
- nonane.ent
- decane.ent

First, let's revisit redirection...

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

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

Instead, we can do...

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

Note the double >'s – the append' operator



data

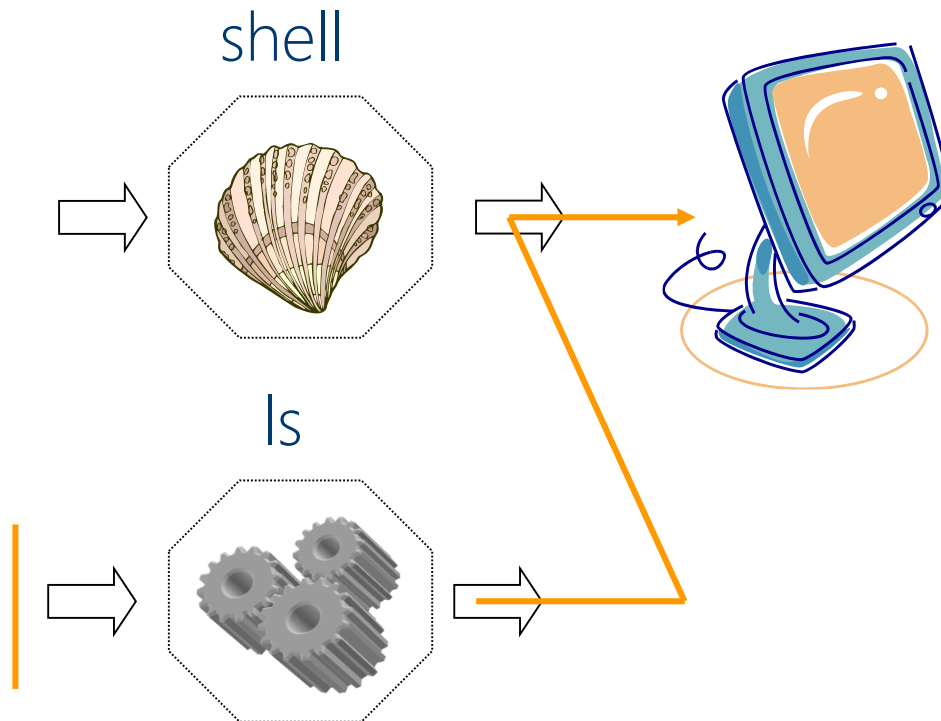
- cubane.pdb
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- methane.pdb
- octane.pdb
- pentane.pdb
- propane.pdb
- butane.ent
- heptane.ent
- hexane.ent
- nonane.ent
- decane.ent

We know that...

Normally, standard output is directed to a display:

We know that...

Normally, standard output is directed to a display:

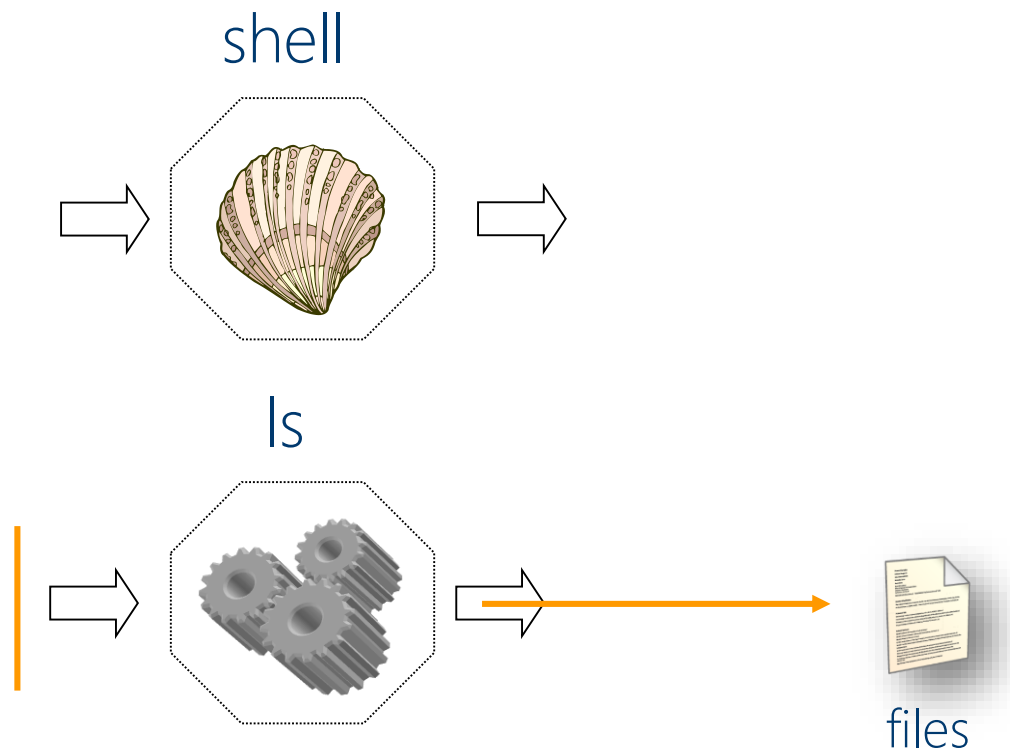




We know that...

Normally, standard output is directed to a display:

But we have redirected it to a file instead:



But what happens with error messages?

But what happens with error messages?

For example...

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

But what happens with error messages?

For example...

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

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

But what happens with error messages?

For example...

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

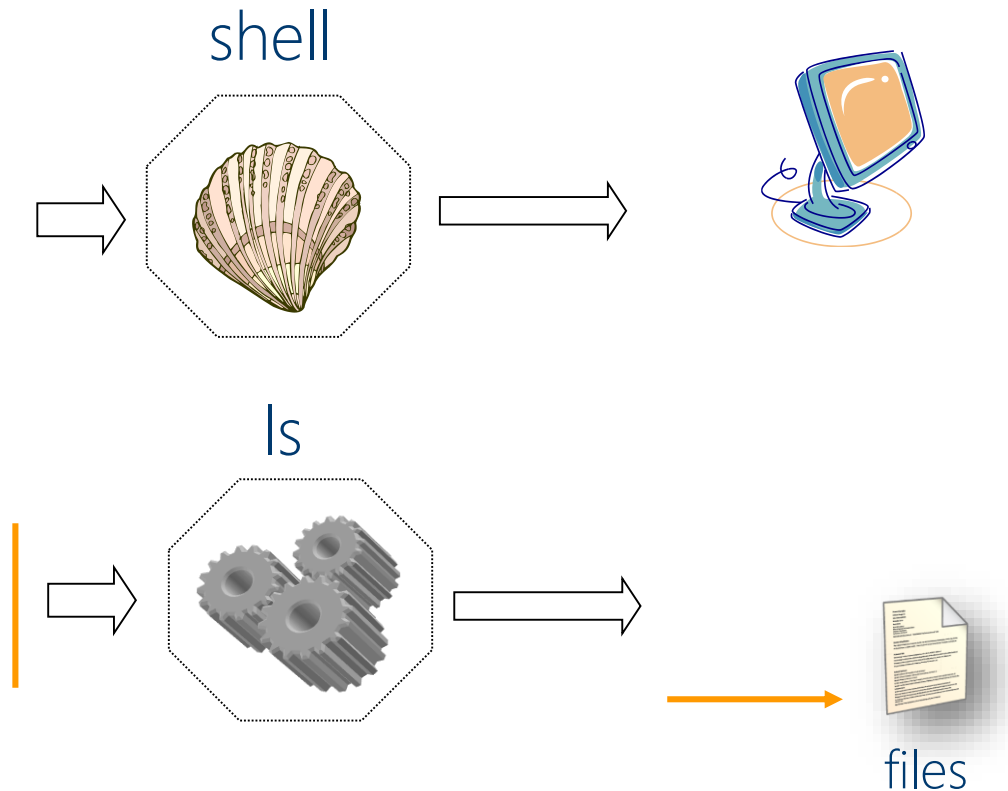
No files are listed in *files*, as you might expect.

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

This is because error messages are sent to the standard error (stderr), separate to stdout

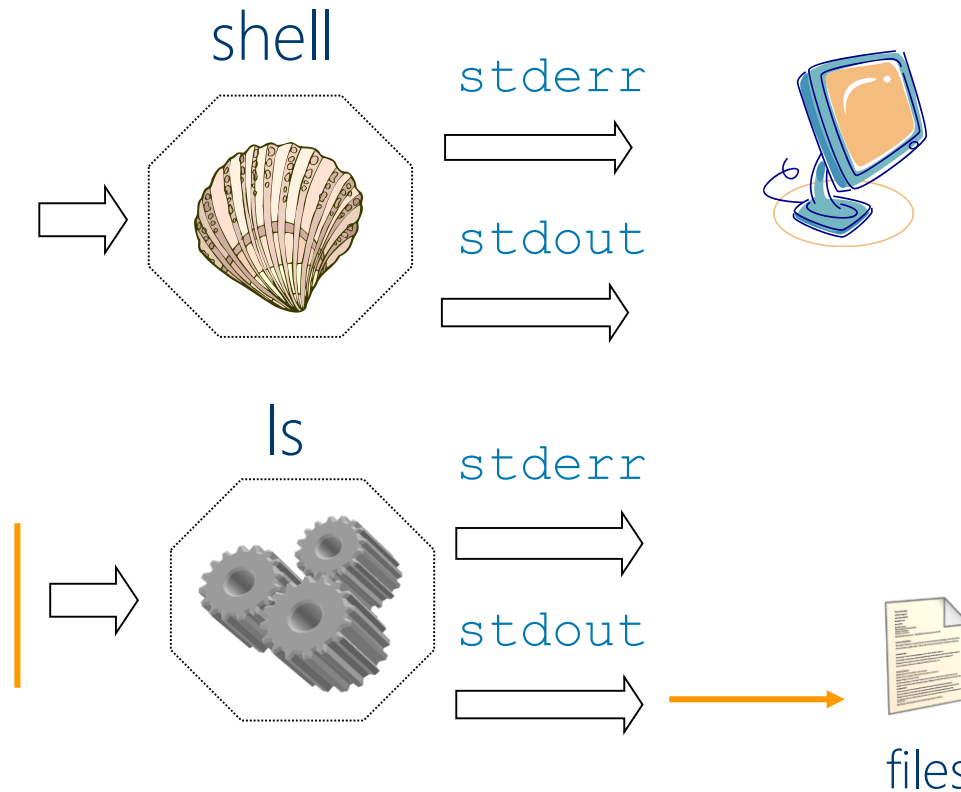
This is because error messages are sent to the standard error (stderr), separate to stdout

So what was happening with the previous example?



This is because error messages are sent to the standard error (stderr), separate to stdout

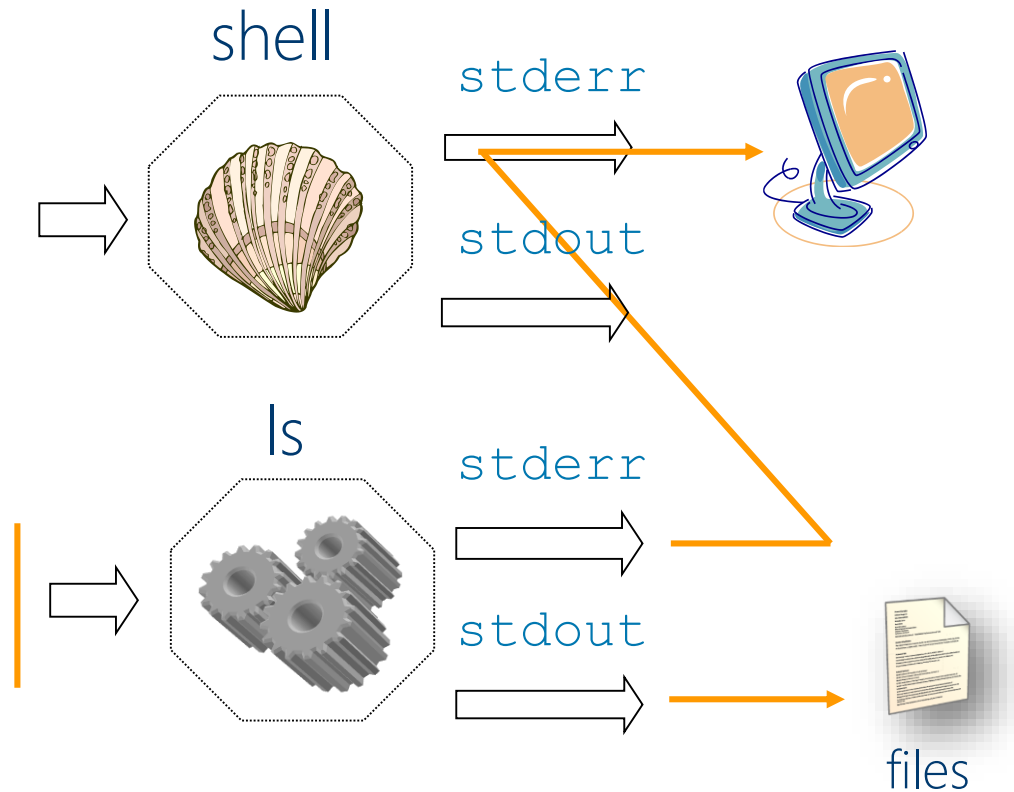
So what was happening with the previous example?





This is because error messages are sent to the standard error (stderr), separate to stdout

So what was happening with the previous example?



We can capture standard error as well as standard output

We can capture standard error as well as standard output

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

We can capture standard error as well as standard output

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

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

Now we have any error messages stored in error-log

We can capture standard error as well as standard output

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

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

Now we have any error messages stored in error-log

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

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

We can capture standard error as well as standard output

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

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

Now we have any error messages stored in error-log

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

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



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

We can capture standard error as well as standard output

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

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

Now we have any error messages stored in error-log

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
```

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
```

Refers to  
stdout

Refers to  
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

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:

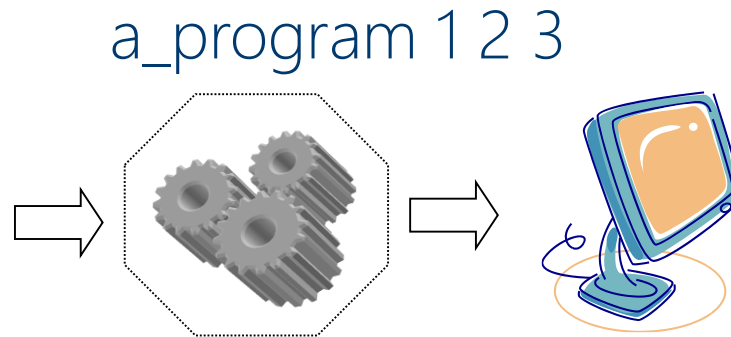
```
$ ls /usr /some/nonexistent/path 1>> files
2>> error-log
```

>	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

We've seen how pipes and filters work with using a single program on some input data...

We've seen how pipes and filters work with using a single program on some input data...



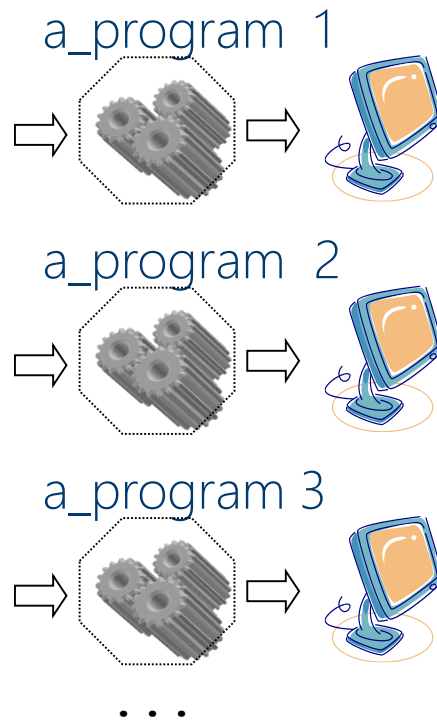


We've seen how pipes and filters work with using a single program on some input data...

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

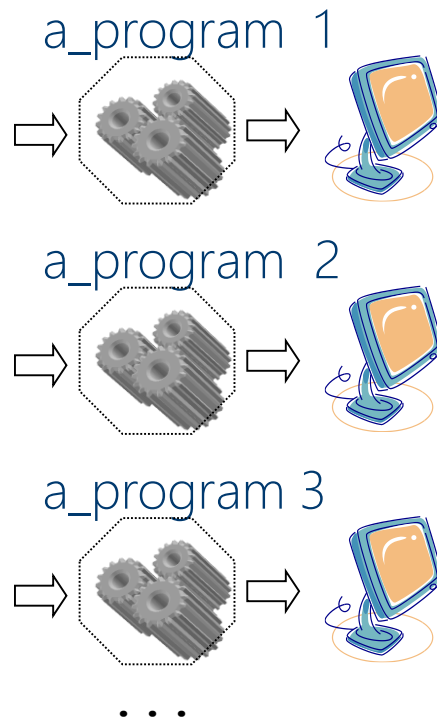
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But what about running the same program *separately*, for each input?



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

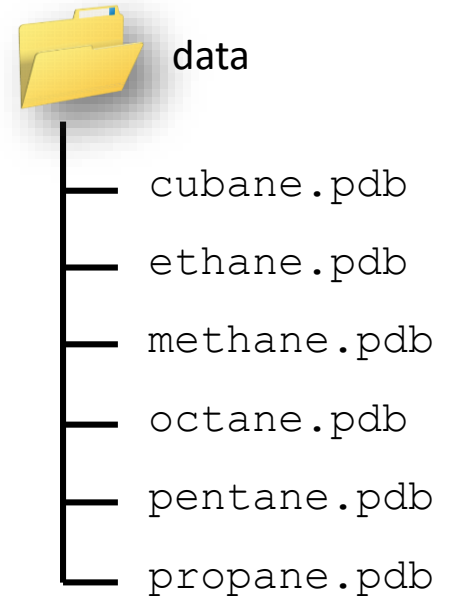


We can use *loops* for this...

So what can we do with loops?

So what can we do with loops?

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

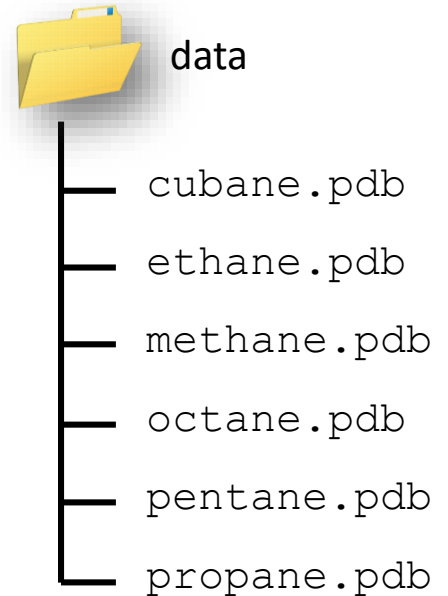


So what can we do with loops?

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%)
```



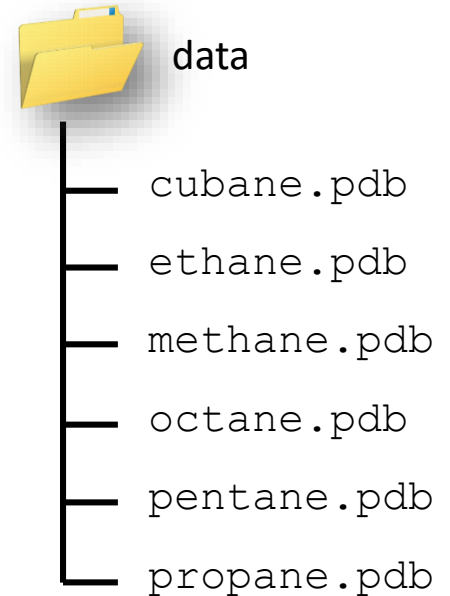
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We could do the following for each:

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

← typical output  
from the zip  
command



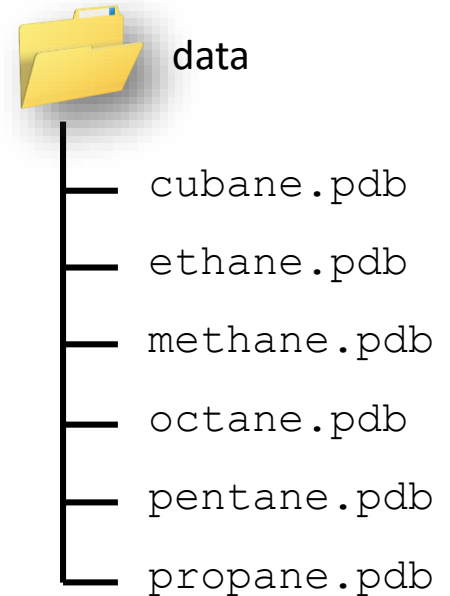
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The zip file we  
wish to create



← typical output  
from the zip  
command



So what can we do with loops?

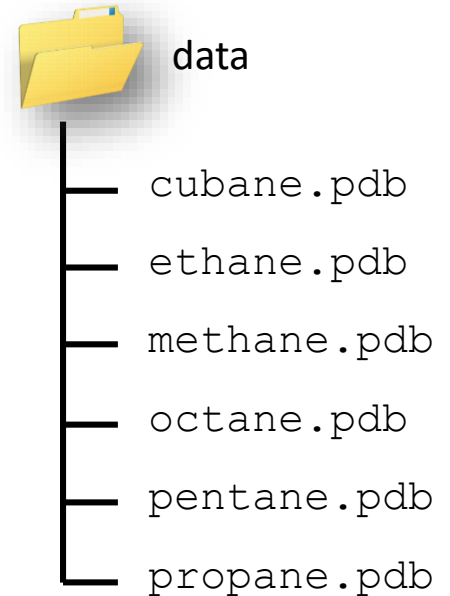
Let's go back to our first set of pdb files, and assume we want to compress each of them

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

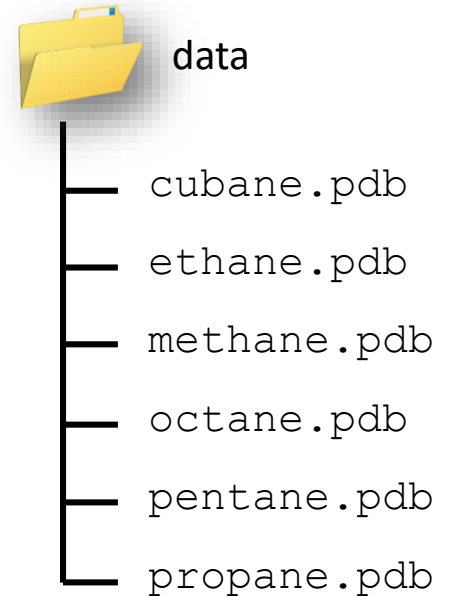
So what can we do with loops?

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We could do the following for each:

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

Not efficient for many files



Using a loop, we can iterate over each file,  
and run zip on each of them:

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

Using a loop, we can iterate over each file,  
and run *zip* on each of them:

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



For each pdb file in  
this directory...

Using a loop, we can iterate over each file,  
and run *zip* on each of them:

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

Run this command

Using a loop, we can iterate over each file,  
and run *zip* on each of them:

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



This is the end  
of the loop

Using a loop, we can iterate over each file,  
and run *zip* on each of them:

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

A diagram illustrating the loop construct. Two purple rectangular boxes highlight the semicolons in the command. Two blue lines originate from these boxes and point downwards towards the explanatory text.

The semicolons separate each  
part of the loop construct

Using a loop, we can iterate over each file,  
and run *zip* on each of them:

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

This expands to a list of every  
pdb file



Using a loop, we can iterate over each file,  
and run *zip* on each of them:


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



This expands to a  
list of every pdb file

Using a loop, we can iterate over each file,  
and run *zip* on each of them:

```
$ 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

Using a loop, we can iterate over each file,  
and run *zip* on each of them:

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

We reference the 'file' variable  
again

Using a loop, we can iterate over each file,  
and run *zip* on each of them:

```
$ 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%)
```

Using a loop, we can iterate over each file,  
and run *zip* on each of them:

```
$ 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%)
```

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

Using a loop, we can iterate over each file, and run *zip* on each of them:

```
$ 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%)
```

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

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

Now instead, what if we wanted to output the first line of each pdb file?

Now instead, what if we wanted to output the first line of each pdb file?

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

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

```
==> ethane.pdb <==  
COMPND      ETHANE
```

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

...



Now instead, what if we wanted to output the first line of each pdb file?

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

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

← head produces this  
(it's not in the file)

```
==> ethane.pdb <==  
COMPND      ETHANE
```

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

...

Now instead, what if we wanted to output the first line of each pdb file?

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

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

```
==> ethane.pdb <==  
COMPND      ETHANE
```

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

...

head produces this  
(it's not in the file)

this is actually the first  
line in this file!

Now instead, what if we wanted to output the first line of each pdb file?

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

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

```
==> ethane.pdb <==  
COMPND      ETHANE
```

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

...

head produces this  
(it's not in the file)

this is actually the first  
line in this file!

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
```

What if we wanted this list sorted in reverse afterwards?



What if we wanted this list sorted in reverse afterwards?


Simple!

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

What if we wanted this list sorted in reverse afterwards?

Simple!

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



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

What if we wanted this list sorted in reverse afterwards?

Simple!

```
$(for file in ls *.pdb; do head -1 $file; done) | sort -r  
COMPND      PROPANE  
COMPND      PENTANE  
COMPND      OCTANE  
COMPND      METHANE  
COMPND      ETHANE  
COMPND      CUBANE
```

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

---

# Checkpoint 5



- Please complete the *What is Model Survey Results*:
  - Blackboard > Course Content > Week 3 (Sept. 28- Oct. 2) > Monday Sept. 28 > Checkpoint 5



# The Unix Shell

## The Secure Shell

Created by Elango Cheran



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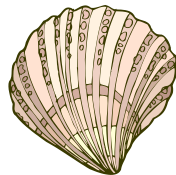




```
$ pwd
```



shell

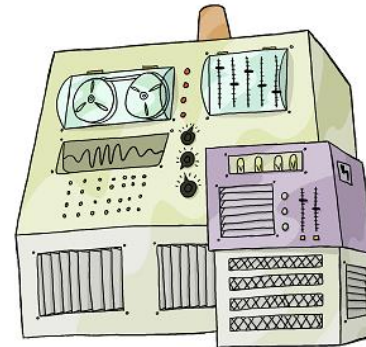
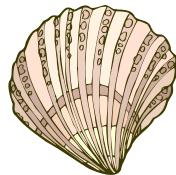




```
$ pwd  
/users/vlad  
$
```



shell



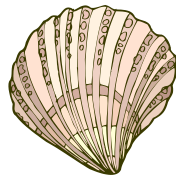




```
login as: vlad  
Password: *****(*)****
```



shell

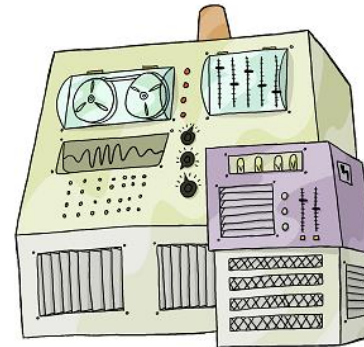
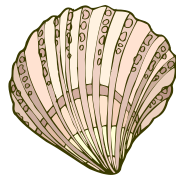




```
login as: vlad  
Password: ****  
$
```



shell

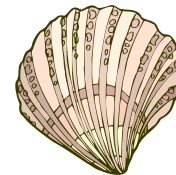
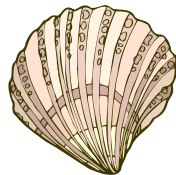




```
login as: vlad  
Password: ****  
moon>
```



shell



remote shell

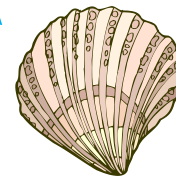
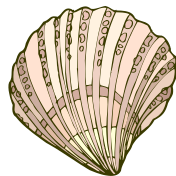




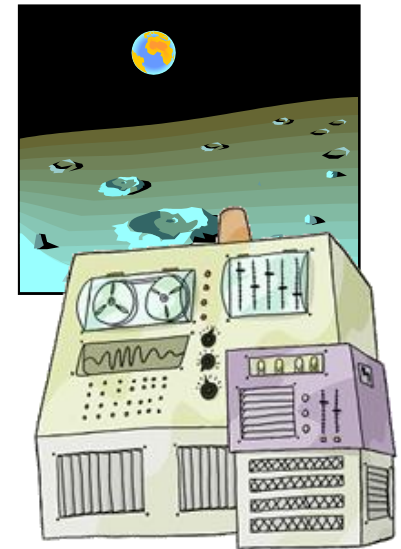
```
login as: vlad  
Password: ****  
moon>
```



shell



remote shell



```
$ pwd
```

```
/users/vlad
```

```
$ ssh vlad@moon
```

**Password:**

```
$ pwd
```

```
/users/vlad
```

```
$ ssh vlad@moon
```

```
Password: ***
```

```
Access denied
```

```
Password:
```

```
$ pwd
```

```
/users/vlad
```

```
$ ssh vlad@moon
```

```
Password: ***
```

```
Access denied
```

```
Password: *****
```

```
moon> pwd
```

```
/home/vlad
```

```
moon> ls -F
```

```
bin/          cheese.txt    dark_side/    rocks.cfg
```

```
$ pwd
```

```
/users/vlad
```

```
$ ssh vlad@moon
```

```
Password: ***
```

```
Access denied
```

```
Password: *****
```

```
moon> pwd
```

```
/home/vlad
```

```
moon> ls -F
```

```
bin/          cheese.txt    dark_side/    rocks.cfg
```

```
moon> exit
```

```
$ pwd
```

```
/users/vlad
```



```
$ ssh vlad@moon
```

```
Password: ****
```

```
moon> pwd
```

```
/home/vlad
```

```
moon> ls -F
```

```
bin/      cheese.txt  dark_side/  rocks.cfg
```

```
moon> exit
```

```
$ pwd
```

```
/users/vlad
```

```
$ ls -F
```

```
bin/          data/      mail/      music/
notes.txt     papers/    pizza.cfg  solar/
solar.pdf     swc/
```

```
$ scp vlad@moon:/home/vlad/cheese.txt  
      vlad@earth:/users/vlad
```

source file...

```
$ scp vlad@moon:/home/vlad/cheese.txt  
    vlad@earth:/users/vlad
```



source file...

...to destination directory

```
$ scp vlad@moon:/home/vlad/cheese.txt  
    vlad@earth:/users/vlad
```

source file...

...to destination directory

source and destination are written as

user@computer:path

```
$ scp vlad@moon:/home/vlad/cheese.txt  
      vlad@earth:/users/vlad
```

```
Password:  *****
```

```
cheese.txt                                100%  9  1.0 KB/s  00:00
```

```
$ scp vlad@moon:/home/vlad/cheese.txt  
      vlad@earth:/users/vlad
```

```
$ scp -r vlad@moon:/home/vlad/dark_side  
      vlad@earth:/users/vlad
```

 -r indicates a directory and its contents

```
$ scp -r vlad@moon:/home/vlad/dark_side  
    vlad@earth:/users/vlad
```

```
$ scp -r vlad@moon:/home/vlad/dark_side  
    /users/vlad
```

```
$ pwd  
/users/vlad
```

```
$ scp -r vlad@moon:/home/vlad/dark_side  
    .
```

same destination path



```
$ ssh vlad@moon
```

```
Password:  *****
```

```
moon> df -h
```

<i>Filesystem</i>	<i>Size</i>	<i>Used</i>	<i>Avail</i>	<i>Use%</i>	<i>Mounted On</i>
<i>/dev/sda1</i>	<i>7.9G</i>	<i>2.1G</i>	<i>5.5G</i>	<i>28%</i>	<i>/</i>
<i>/dev/sda2</i>	<i>791G</i>	<i>150G</i>	<i>642G</i>	<i>19%</i>	<i>/home</i>

```
moon> df -h > usage.txt
```

```
moon> exit
```

```
$ scp vlad@moon:/home/vlad/usage.txt .
```

```
Password:  *****
```

```
usage.txt                                100%   134   1.0 KB/s   00:00
```



```
$ ssh vlad@moon 'df -h'
```

**Password:** \*\*\*\*\*

<i>Filesystem</i>	<i>Size</i>	<i>Used</i>	<i>Avail</i>	<i>Use%</i>	<i>Mounted On</i>
<i>/dev/sda1</i>	<i>7.9G</i>	<i>2.1G</i>	<i>5.5G</i>	<i>28%</i>	<i>/</i>
<i>/dev/sda2</i>	<i>791G</i>	<i>150G</i>	<i>642G</i>	<i>19%</i>	<i>/home</i>

```
$ ssh vlad@moon 'df -h'
```

**Password:** \*\*\*\*\*

Filesystem	Size	Used	Avail	Use%	Mounted On
/dev/sda1	7.9G	2.1G	5.5G	28%	/
/dev/sda2	791G	150G	642G	19%	/home

```
$ ssh vlad@moon 'df -h' >> usage.log
```

**Password:** \*\*\*\*\*

```
$ ls -F
```

bin/	data/	mail/	music/
notes.txt	papers/	pizza.cfg	solar/
solar.pdf	swc/	usage.log	usage.txt

same result

character stream



```
$ echo "open sesame, please" | ssh  
    vlad@moon 'cat > magic.txt'
```

**Password:** \*\*\*\*

character stream

remote shell receives stream from pipe

```
$ echo "open sesame, please" | ssh  
    vlad@moon 'cat > magic.txt'
```

**Password:** \*\*\*\*\*

redirection within remote shell

remote command receives input piped to ssh  
cat repeats input stream as output

```
graph LR; A["character stream"] --> B["$ echo \"open sesame, please\" | ssh"]; B --> C["remote shell receives stream from pipe"]; C --> D["remote command receives input piped to ssh"]; D --> E["cat repeats input stream as output"]; E --> F["redirection within remote shell"];
```

```
$ ssh vlad@moon 'ls -F /home/vlad'
```

```
Password: ****
```

```
bin/      cheese.txt    dark_side/  rocks.cfg
```

before

```
$ echo "open sesame, please" | ssh
```

```
    vlad@moon 'cat > magic.txt'
```

```
Password: ****
```

```
$ ssh vlad@moon 'ls -F /home/vlad'
```

```
Password: ****
```

```
bin/      cheese.txt    dark_side/
```

```
magic.txt
```

after

```
rocks.cfg
```

```
$ ssh vlad@moon 'ls -F /home/vlad'
```

```
Password: ****
```

```
bin/      cheese.txt    dark_side/  rocks.cfg
```

} before

```
$ echo "open sesame, please" | ssh
```

```
    vlad@moon 'cat > magic.txt'
```

```
Password: ****
```

```
$ ssh vlad@moon 'ls -F /home/vlad'
```

```
Password: ****
```

```
bin/      cheese.txt    dark_side/  magic.txt
```

} after

```
rocks.cfg
```

```
$ scp vlad@moon:/home/vlad/magic.txt .
```

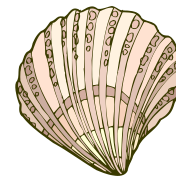
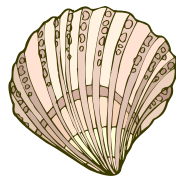
```
Password: ****
```



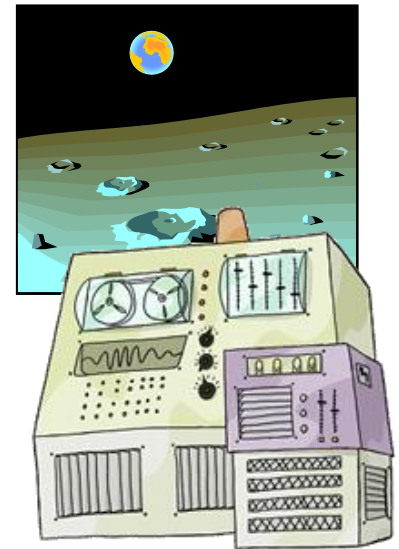
```
login as: vlad  
Password: ****
```



shell



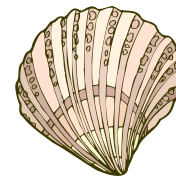
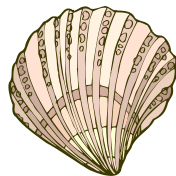
remote shell



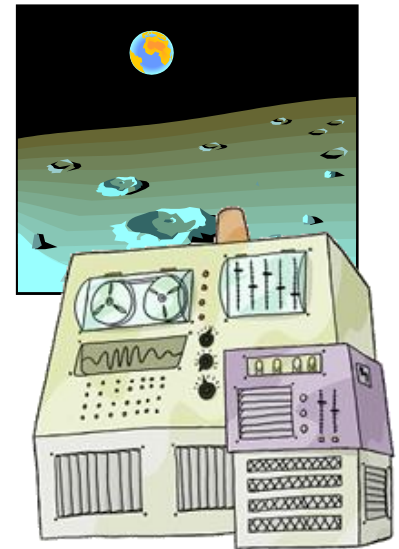


```
login as: vlad  
Password: thriller
```

shell



remote shell



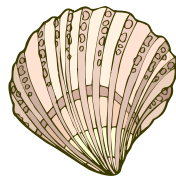




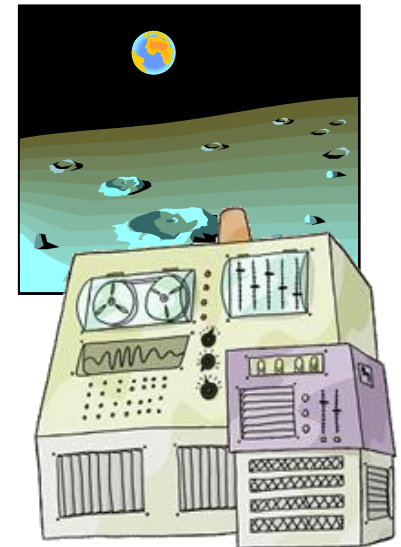
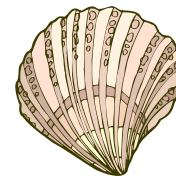
```
login as: vlad  
Password: thriller
```

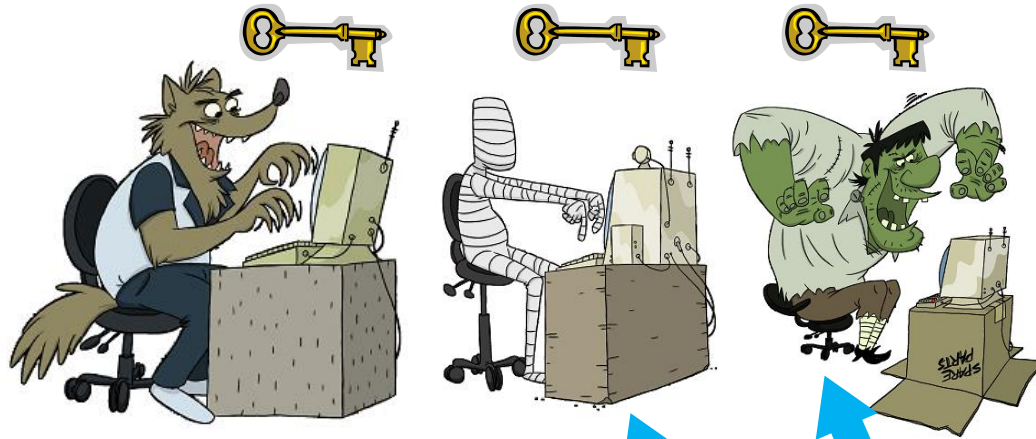


shell

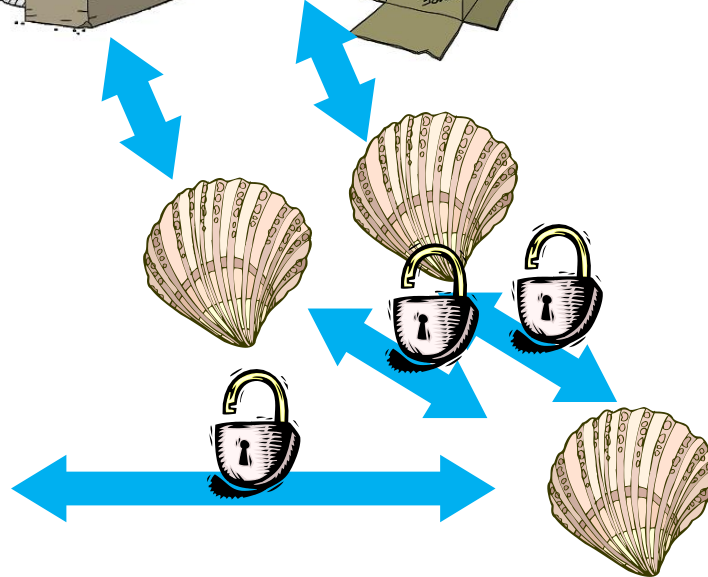
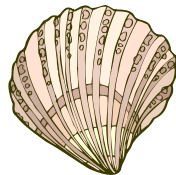


remote shell

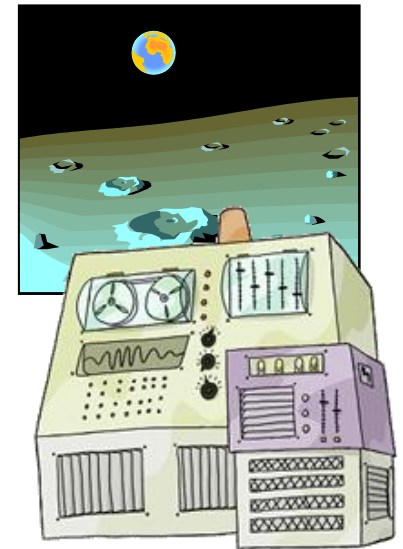


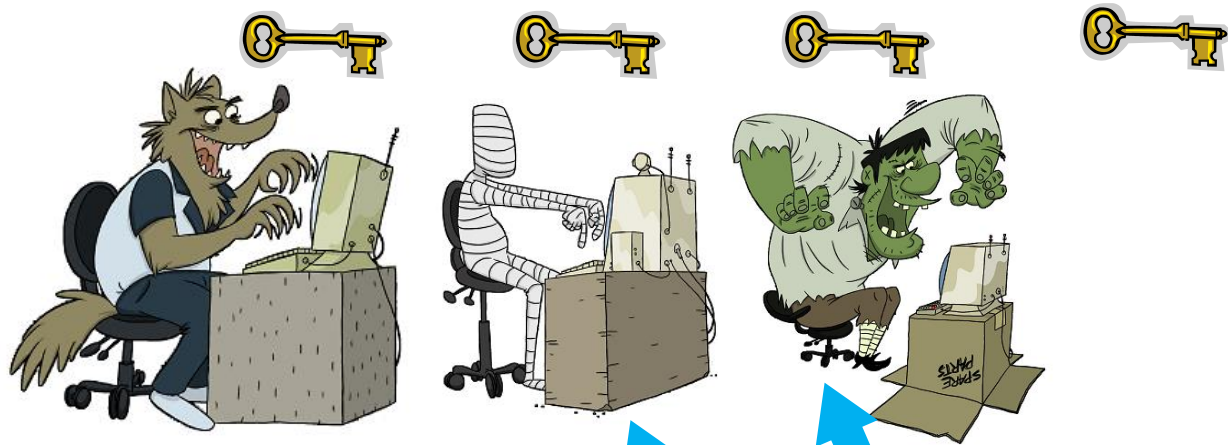


shell

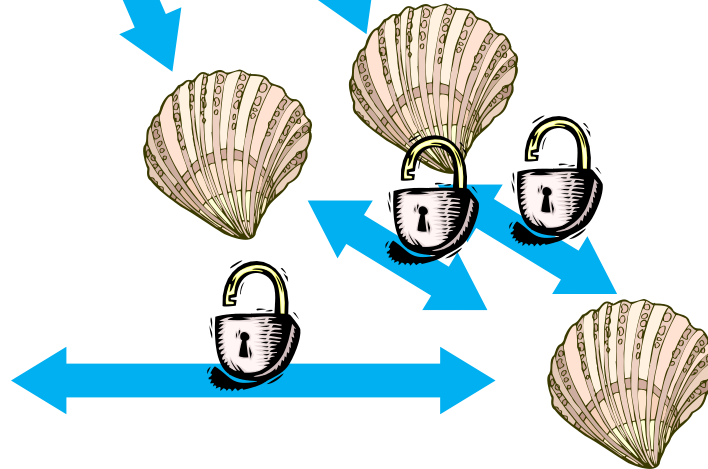
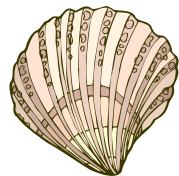


remote shell

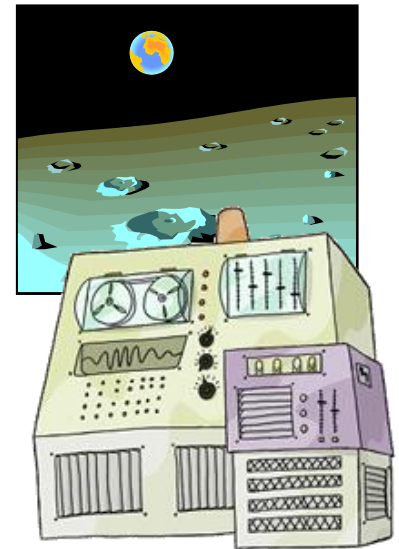


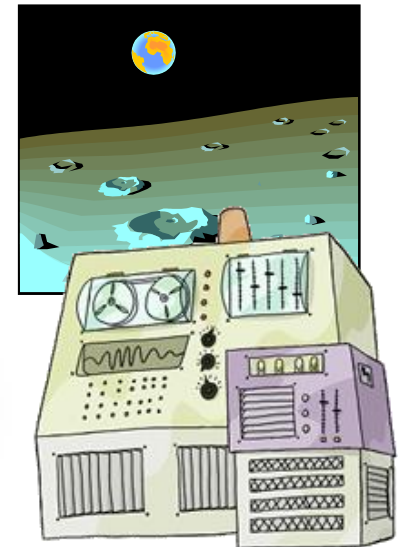
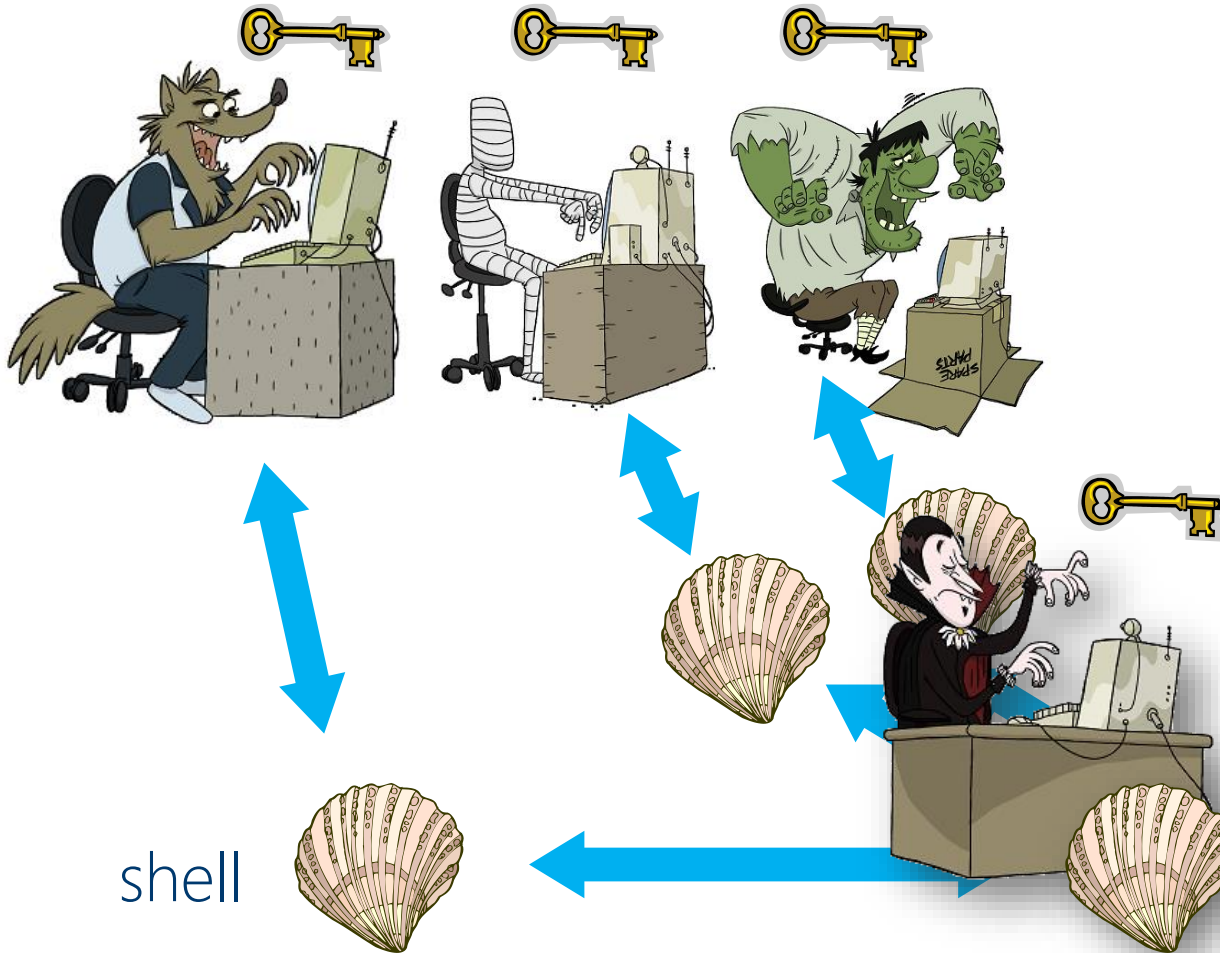


shell



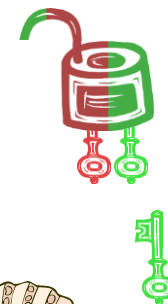
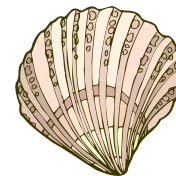
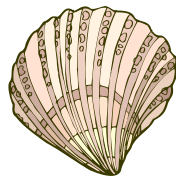
remote shell







shell

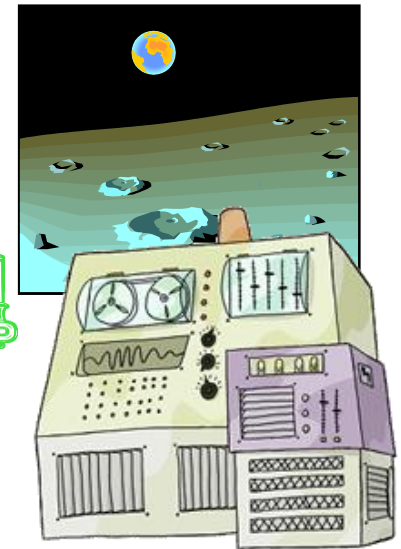
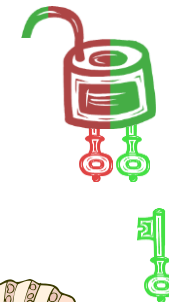
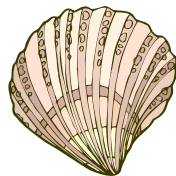


remote shell

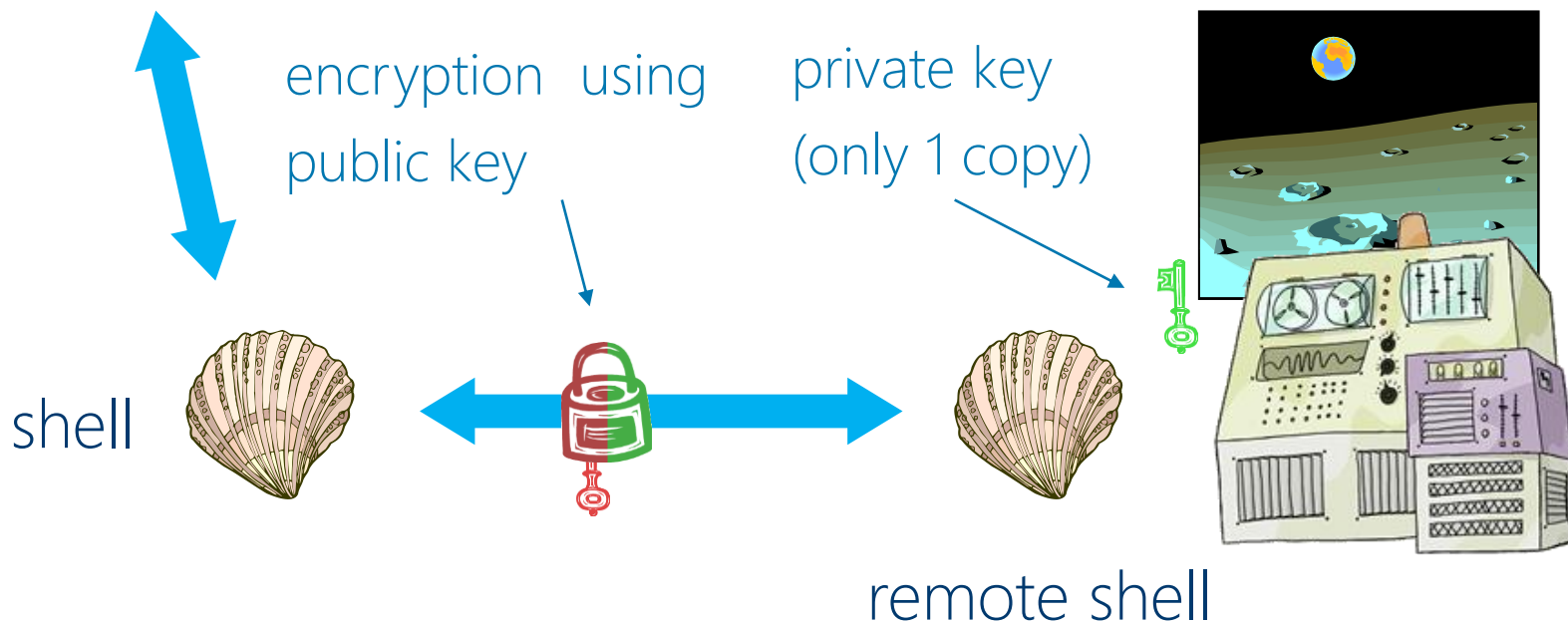
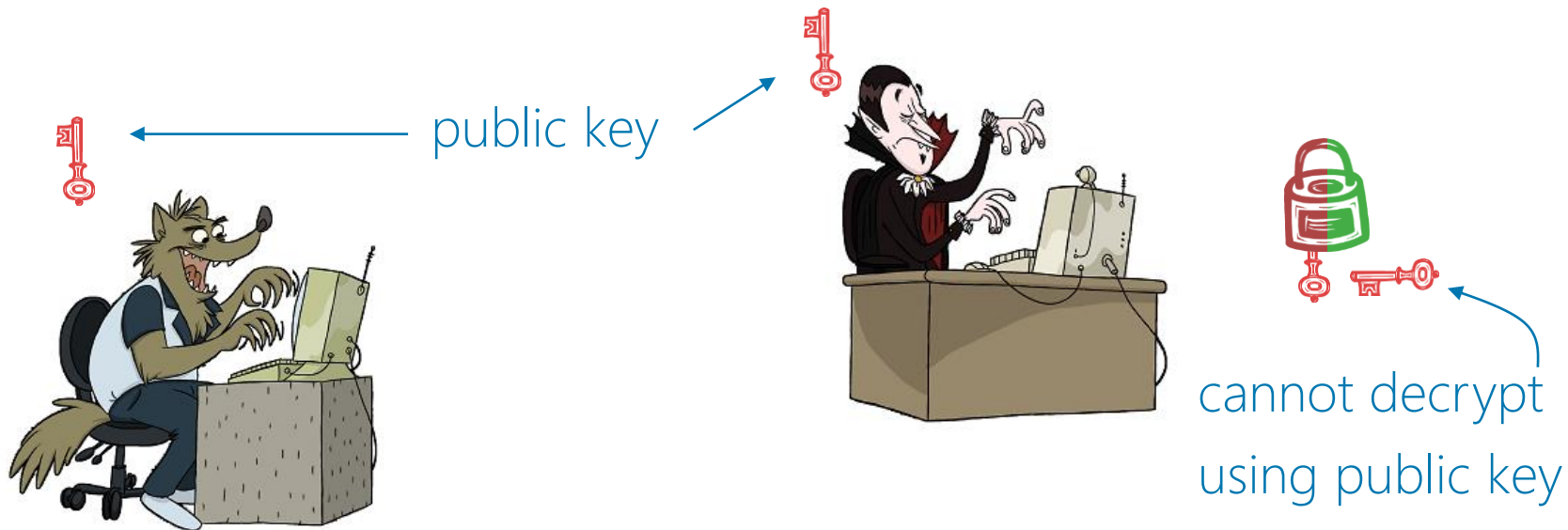


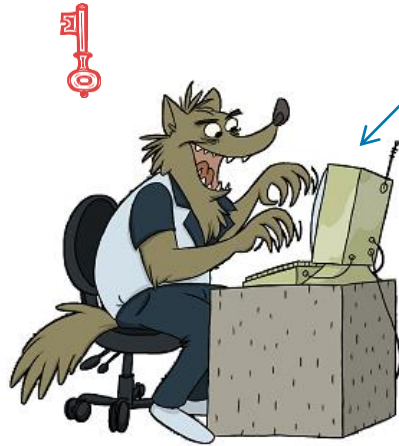


shell



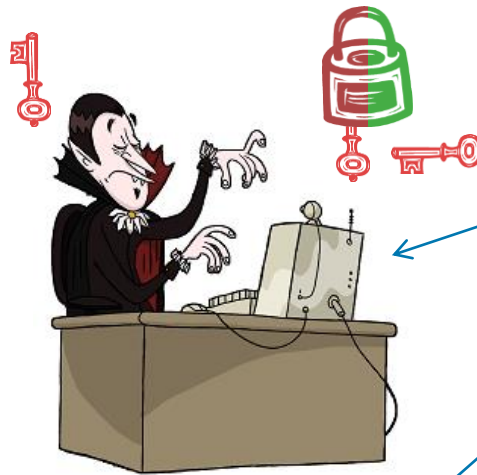
remote shell





login as: vlad

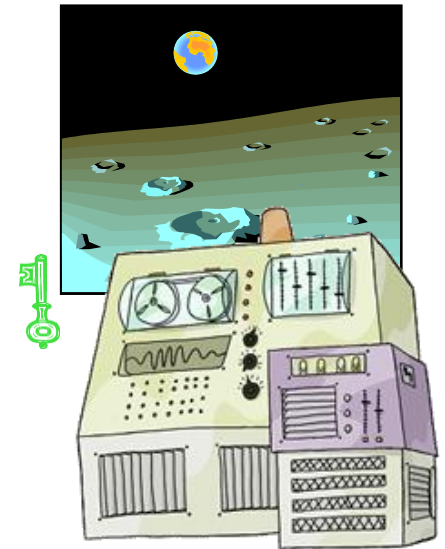
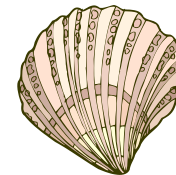
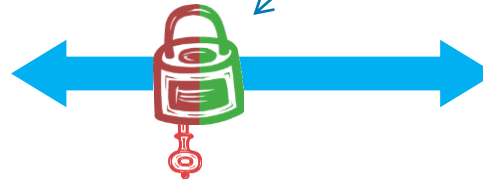
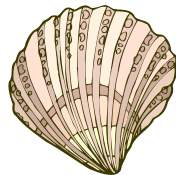
Password: \*\*\*\*



huxyo ew: xdvw

uqfcmjbn: lhiujdbj

shell



remote shell



```
$ ssh vlad@moon
```

```
The authenticity of host 'moon (10.1.2.3) '  
can't be established.
```

```
RSA key fingerprint is
```

```
f1:68:f5:90:47:dc:a8:e9:62:df:c9:21:f0:8b:c5:39.
```

```
Are you sure you want to continue connecting  
(yes/no) ? yes
```

```
Warning: Permanently added 'moon,10.1.2.3' (RSA)  
to the list of known hosts.
```

```
Password: *******
```

```
moon>
```

```
while true:
    ...
    if time.mins == 30:
        ssh vlad@moon 'df -h' >> usage.log
    ...
```

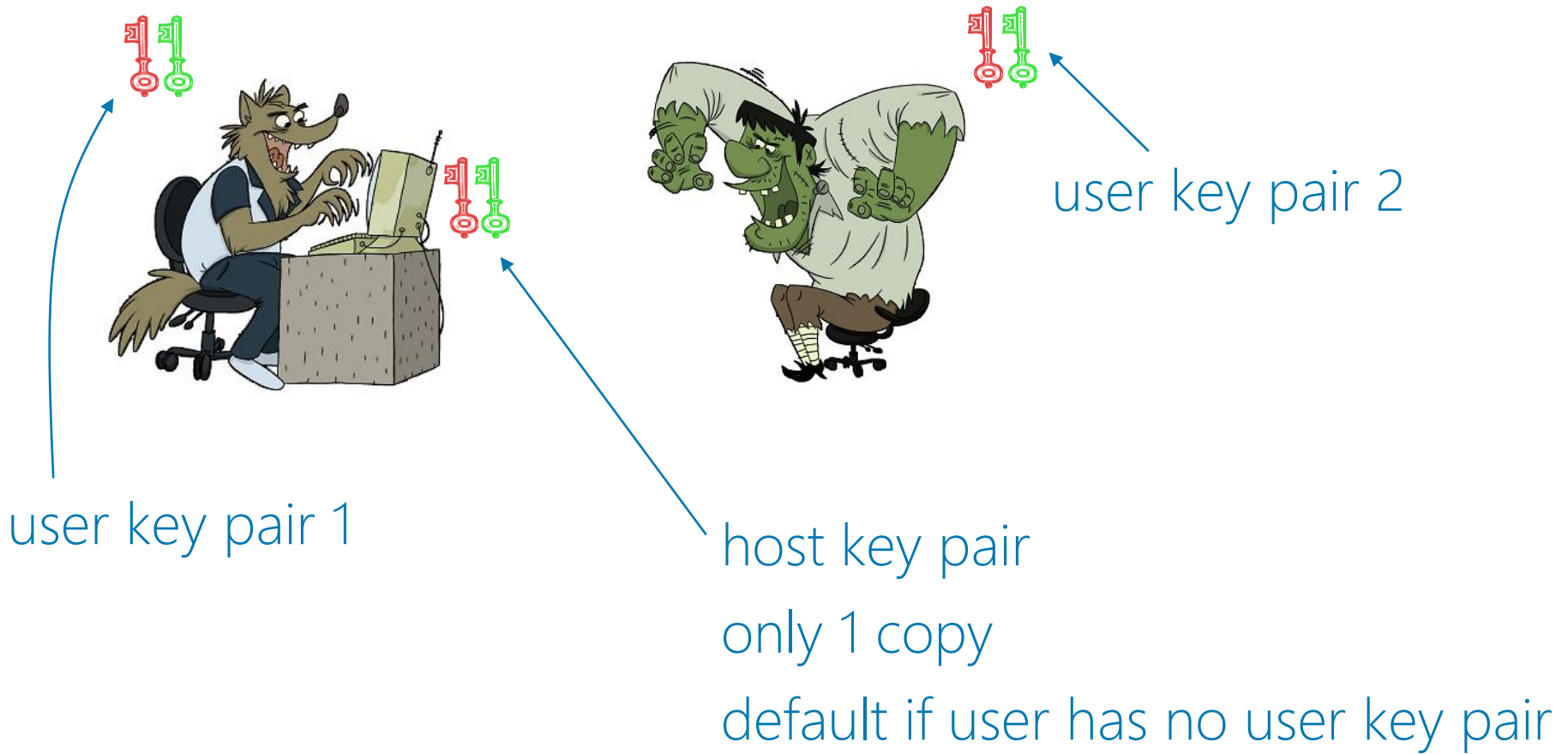
```
while true:
    ...
    if time.mins == 30:
        ssh vlad@moon 'df -h' >> usage.log
    ...
```

```
$ ssh vlad@moon 'df -h' >> usage.log
```

**Password:**

*Connection closed by 10.1.2.3* ← waited too long

\$



```
$ ssh-keygen -t rsa
```

*Generating public/private rsa key pair.*

**Enter file in which to save the key**

**(/users/vlad/.ssh/id\_rsa):** ← press enter

**Enter passphrase (empty for no**

**passphrase):** \*\*\*\*\*

**Enter same passphrase again:** \*\*\*\*\*

Your identification has been saved in  
/users/vlad/.ssh/id\_rsa.

Your public key has been saved in  
/users/vlad/.ssh/id\_rsa.pub.

The key fingerprint is:

d3:1a:27:38:aa:54:e8:a5:03:db:79:2f:b2:c3:c9:3d

```
$ ssh vlad@moon
```

**Enter passphrase for key**

```
'/users/vlad/.ssh/id_rsa': ****
```

```
moon>
```

```
$ ssh-keygen -t rsa
```

*Generating public/private rsa key pair.*

**Enter file in which to save the key**

**(/users/vlad/.ssh/id\_rsa):** ← press enter

**Enter passphrase (empty for no passphrase):** ↗

**Enter same passphrase again:** ↘

Your identification has been saved in  
/users/vlad/.ssh/id\_rsa.

Your public key has been saved in  
/users/vlad/.ssh/id\_rsa.pub.

The key fingerprint is:

d3:1a:27:38:aa:54:e8:a5:03:db:79:2f:b2:c3:c9:3d

```
$ scp ~/.ssh/id_rsa.pub vlad@moon
```

```
Password:  *****
```

```
$ ssh vlad@moon
```

```
Password:  *****
```

```
moon> cat id_rsa.pub >> ~/.ssh/authorized_keys
```

```
moon> exit
```

```
$ cat ~/.ssh/id_rsa.pub | ssh vlad@moon
```

```
'cat >> ~/.ssh/authorized_keys'
```

```
Password:  *****
```

```
$ ssh-copy-id vlad@moon
```

```
Password:  *****
```



```
$ ssh vlad@moon
```

```
moon>
```



```
while true:
```

```
...
```

```
if time.mins == 30:
```

```
    ssh vlad@moon 'df -h' >> usage.log
```

```
...
```

# Checkpoint 6



- Please answer the *Self-Assessment* :
  - Blackboard > Course Content > Week 3 (Sept. 28- Oct. 2) > Monday Sept. 28 > Checkpoint 6



# QOTD

- All models are wrong, but some are useful

Geroge Box  
(1919–2013)  
British statistician

