

VASP WORKSHOP AT NCHC

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Lecture Notes

Hands-on session 2

Lecturer : T. C. Leung
Department of Physics
National Chung Cheng University

Outline

- 進入Unit世界
- 編輯器vi
- Fortran 77
- xmgrace
- vaspview

進入Unit世界

Login:guest ←account name

Password:***** (abcdef) ←password

更改密碼 % passwd

一些常用之指令

% pwd (顯示現在所在之目錄)

/user/leung/lapw/cu

% cd ../Fe (改變目錄)

% ls *.f (列出所有 *.f 之 files)

% ls -l (long list)

% ls -l

```
-rwxrwxrwx  1 users user 4564 Jun11 20:45 love
dr--r-----  2 users user  547 Jun11 22:50 sub/
-rw-rw-r--  1 users user 4135 Jun21 11:20 t1
  ↑  ↑  ↑           ↑   ↑   ↑       ↑           ↑
  u  g  o         owner group 大小   時間       名稱
```

% chmod u+x filename

% chmod 741 filename

% ls-a (將隱藏檔案列出, eg .csrch .login)

% ls-F (將可執行之檔後加*,目錄加/)

```
love  ppd*  t1*  sub/  test/
```

0	000	---
1	001	--x
2	010	-w-
3	011	-wx
4	100	r--
5	101	r-x
6	110	rw-
7	111	rwX

% mkdir dname

% rmdir dname

% rm filename (刪除filename)

% mv filename1 filename2 (改名)

% cp [-i p r] filename target (複製)

i:要確認

p:保留原時間

r:複製子目錄

% cat filename (>test)

列出filename之內容並將之放入test之中

% move filename

列出filename之內容,每一螢幕停一下

% head -n filename

將filename之前 n 行列出

% tail -n filename (>>test)

將filename之最後 n 行列出 (並附在 test 後)

% grep -i string filename

從filename找出含string之行, 不計大小寫

% grep 'total energy' filename

% find -name filename -print

尋找filename之所在,並列出其路徑

?,*,[, { }

```
ls hw?      →hw2,hw3,hw4
ls hw??     →hw11,hw12
ls hw*      →hw2,hw3,hw4,hw11,hw12
ls hw[2-11] →hw2,hw3,hw4,hw11
ls hw{2,12} →hw2,hw12
ls test[a-c] →testa,testb,testc
```

alias

```
alias la ls-a ;
alias ch1 'cd /usr/john ; ls-l'
alias rm 'rm -i';
alias hm 'history | more '
```

unalias

```
Unalias ch1
```

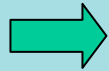
欲看目前已有之別名定義,可鍵入alias

編輯器vi

% vi filename

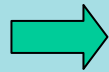
There are 2 modes in vi editor : (1) insert mode, (2) command mode

i,a,o,I,A,O



insert mode (鍵入字元(內容))

ESC



command mode (執行命令)

h(←), j(↓), k(↑), l(→)

nG

到第n行

G

到最後一行

^g

顯示游標所在之行數

^f

視窗下移一螢幕

^b

視窗上移一螢幕

x	刪除游標所在之字元
dd	刪除一行
ndd	刪除n行
u	undo 上一命令
p,P	貼回
/string	找字串
:q!	quit
:zz	存檔(原名)
:w! filename	存檔為filename
:set ic	忽略大小寫
:set nu	列出行數
:1,\$ s/string1/string2/g	更改字串
:n1,n2 w! filename	將n1到n2行寫入
:r filename	讀入filename

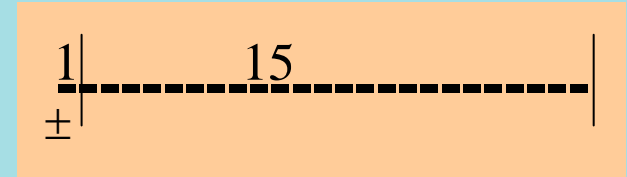
Fortran 77

integer : single precision 2 Bytes (16 bits)

$$\pm 32767 \quad (2^{15} - 1 \rightarrow -2^{15} + 1)$$

double precision 4 bytes (32 bits)

$$\pm 2147483647 \quad (2^{31} - 1 \rightarrow -2^{31} + 1)$$



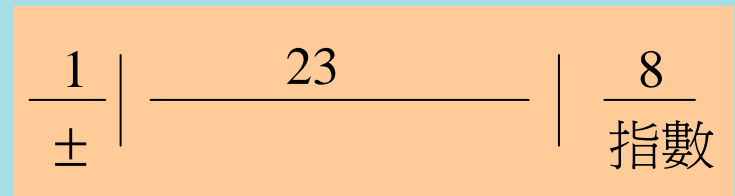
real : single precision 4 Bytes (32 bits)

有效位數為 6~8

$$\text{min} : 1.18 \times 10^{-38} \quad \text{max} : 3.4 \times 10^{38}$$

double precision 8 Bytes (64 bits)

$$\text{有效位數為 } 15 \sim 16 ; \quad \text{min} : 2.23 \times 10^{-308} \quad \text{max} : 1.79 \times 10^{308}$$



character : 用 1 Byte (8bits $2^7 - 1 = 127$) 代表一個字元

(A,B,...,Z,a,b,c, ... ,z,1,2,3, ... ,*,?, ...)

Array : A(100) , B(100,10) , IX(10,10,10)

Dimension A(100) , B(100,10) , IX(10,10,10)

parameter (nk=200)

Dimension A(nk,nk) , B(nk,3) , IX(nk,nk,nk)

go to n (.eq. .gt. .lt. .le. .ge. .and. .or.)

if (x.eq.y) go to n

if ((x .eq. y) .and. (I .gt. J)) go to n

if (...) then

A = B

.....

Else

.....

Endif

do n1 j = 1,100

.....

do n2 l = 3,13,2

.....

n2 continue

.....

n1 contunue

c = = = & 第7位開始至第80位(內容) 81

第1位有c表示本行為描述用途

第6位有字表示繼續上一行

```
program test
```

```
open (5,file='a.dat')
```

```
open (6,file='a.out')
```

```
read (5,1) x
```

```
1 format (F10.5)
```

```
y=2*x*cos(x)
```

```
write(6,1) x
```

```
stop
```

```
end
```

real variable: a-h , o - z

integer variables: I,J,K,L,M,N

implicit real*8 (a-h,o-z)

+, -, *, /, **, cos(x), tan(x), sin(x)

exp(x), log(x), abs(x), ...

mod(50,3)=2 (餘數)

3F10.5 , 2a5 , E12.3 , 6x , 4I5

2(F10.5,2x,3I4), 2(2I4\\, 'x=',F10.5)

```
% fort77 -o a.x a.f
```

```
% a.x
```

program example

common /aa/ x,y

common /ab/ b

.....

if (a .eq. b) go to 10

call xxx (a,b,c)

10 z=pot(a)**2+3.5

.....

stop

end

subroutine xxx (a,b,c)

common /aa/ x,y

.....

return

end

Fuction pot(x)

common /ab/ b

pot=x**2+3.0*b

return

end