Tecniche di programmazione in chimica computazionale

Loops and choices

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Do loop

- Construct to repeat instructions within a loop

```
 do i=m,n,l
      instructions
      ...
enddo
```

- *i*, *m*, *n* and *l* are integers
- *l* is optional (default 1)

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- Exit instruction: exit the loop
- Cycle instruction: transfer control to enddo
- Examples do1.f90 and do2.f90

Do while construct

- Loop with exit condition

```
 do while(condition)
      instructions
      ...
enddo
```

- Instructions repeated until the condition (logical expression) is true

Do while construct

- Loop with exit condition

  ```
   do while(condition)
         instructions
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  enddo
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If condition

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```
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    instructions
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- Multiple options

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if (condition 1) then
    instructions 1
    ...
elseif (condition 2) then
    instructions 2
    ...
else
    instructions 3
    ...
endif
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- Also allowed: *if (condition) instruction*

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  if (condition) then
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      ...
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      instructions 1
      ...
  elseif (condition 2) then
      instructions 2
      ...
  else
      instructions 3
      ...
  endif
  ```

- Also allowed: *if (condition) instruction*
- Examples if.f90, exit.f90, repeat.f90, cycle.f90 and nested.f90

Case

- Multiple options

```
 select case (expression)
   case (choice1)
      instructions 1
      ...
   case (choice2)
      instructions 2
      ...
end select
```

Case

- Multiple options

```
 select case (expression)
   case (choice1)
      instructions 1
      ...
   case (choice2)
      instructions 2
      ...
end select
```

- Example case.f90

Examples

- fattoriale.f90

Examples

- fattoriale.f90
- fibonacci.f90

Examples

- fattoriale.f90
- fibonacci.f90
- norma_vettore.f90

Examples

- fattoriale.f90
- fibonacci.f90
- norma_vettore.f90
- prodotto_scalare.f90

Examples

- fattoriale.f90
- fibonacci.f90
- norma_vettore.f90
- prodotto_scalare.f90
- matmul.f90