

Tecniche di programmazione in chimica computazionale

Derived types & pointers

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Derived type

- **User-defined** combination of existing types
type name

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components

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end type name

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- Example **example1.f90**

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- Example **example1.f90**
- Example **example2.f90**

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- Advantages:
 - **Dynamic** management of variables
 - **No *a priori* knowledge** of the size problem
 - **Flexibility** in producing a more efficient program (with caveats)

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- Example **p1.f90**

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- *pointer2 => pointer1*

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- Pointer assignment: *pointer => target*
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- Example **p1.f90**
- *pointer2 => pointer1*
- Example **p2.f90**

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- Example **p3.f90**

- Doing operations and assignments on the **target data**

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Pointer dereferencing

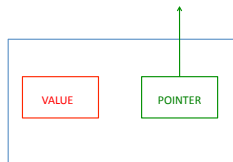
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- Example **p4.f90**

Pointer dereferencing

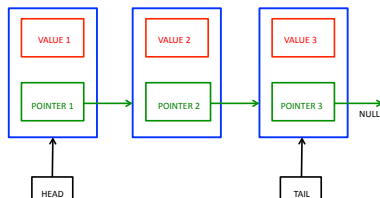
- Doing operations and assignments on the **target data**
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- $p1 = p2 + p3$ means $n1 = n2 + n3$, if $p3 \Rightarrow n3$
- Example **p4.f90**
- Use ***allocate(pointer)*** to create a new data object

Linked list

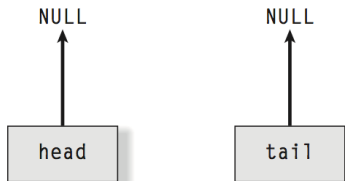
- Derived data type: ordinary variable (integer, real, etc.) + pointer



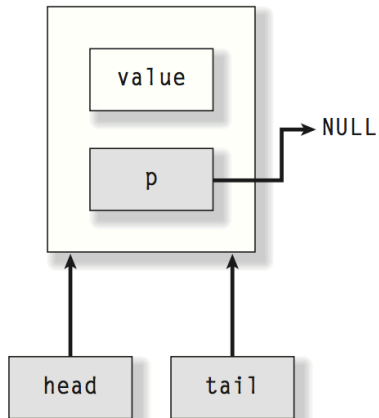
- Linked list



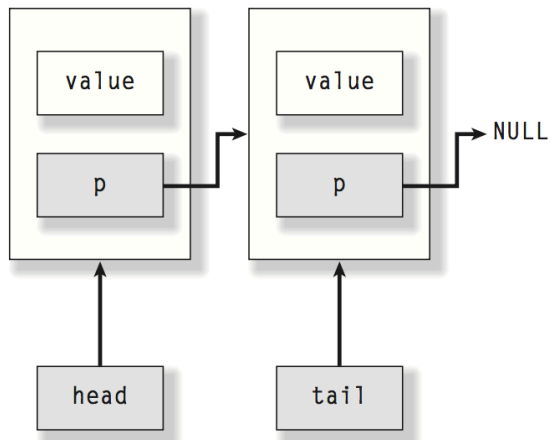
Linked list: first step



Linked list: second step



Linked list: third step



Example `list.f90`