Object-oriented Programming: concepts and Fortran implementation

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Octopus Advanced Courses

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Concepts of object-oriented programming

Programming paradigms

A way to classify programming languages based on their features

- Imperative : instructs the machine how to change its states
  - Procedural
  - **Object-oriented**
- Declarative: programmer declares properties of the desired result, but not how to compute it
  - Functional; Logic; Mathematical; Reactive

Procedural programming

- Based on the concept of the procedure call
- Procedures (routines/subroutines) contain a series of computational steps to be carried out
- Procedures can be call at any point during the execution

Examples: Fortran, ALGOL, COBOL, BASIC, Pascal, C

Procedural programming

- Focus of procedural programming is to break down programming task into a collection of
  - Variables
  - Data structures
  - subroutines

Object-oriented programming (OOP)

- Based on the concept of objects and classes
- Objects contain
  - Data: fields, attributes, or properties
  - Code: procedures or methods

Objects interact with one another

Objects are instances of classes, with a determined type

Example: C++, Java, Python, C#, R, PHP, ….

Object-oriented programming (OOP)

Classes represent broad categories:

- Car
- Dog

Objects represented by the same class share attributes

Cars have a color, dogs have a name and an age, …

Classes serve as a blueprints to create individual objects

Benefits of OOP

- Model complex things as reproducible simple structures → Abstraction
- Reusable
- Polymorphism
- Protect information though encampsulation
- Inheritance

Building blocks

- Classes → user-defined data types
  - A car
- Objects → instance of classes
  - Angel's car
- Methods → represent a behavior/ perform actions
  - Change color, drive, stop
- Attributes → information stored
  - Angel's car is blue

Inheritance

We want to reuse code from other classes

→ Supports re-usability

Child classes automatically gain access to functionalities of their parent class

Example: A *particle* class knows out to give its mass

Child class *charged_particle* directly knows it

Encapsulation

- Notion of public/privated variables
- Protects against common mistakes
- Hide complexity
- Other objects do not have access to the class/ cannot make changes

Example: For a user, a car has a steering wheel, gas and brake. Complexity is hidden in the engine, and the car only exposes simple interfaces.

Abstraction

- Hide complexity
- Extension of encapsulation
- Certain classes are “abstract”. One can only instantiate a child class.

Example: An *animal* does not exist in nature. However, all animals have similar attribute/behavior.

Cat and *dog* are *animals*, and all have a *species* and an *age*. Species and age are common to all animals.

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Polymorphism

- Same method to execute different behavior
- Overriding and overloading (compile time polymorphism)
- Objects of different types can be passed through the same interface
  - → Avoids code duplication

Example: different time propagators behave differently.
But they all do the same task: progate from t to t+dt

prop->propagate(dt)

Object-oriented programming in Fortran

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Fortran vs Fortran 2003

- In “old-fashioned” Fortran: data types and modules
- Features of Fortran 2003:
  - Type-bound procedures
    - *a = c%area()* instead of *a = circle_area(c)*
  - Type extension
    - Allows for inheritance
  - Polymorphism
    - Procedure polymorphism
    - Data polymorphism

OOP in Fortran

- A *type* is a “class”. It can be *abstract* or *extends* from another *type*.
- One can ask the *type* of an object using *select type*
- *Public/private* keywords → data hiding
- Unlimited polymorphic objects are possible
- Multiple inheritance is impossible

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Some details about types in OOP Fortran

- *Abstract* type:

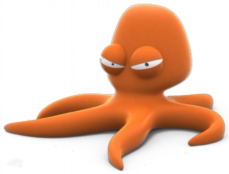
  type that cannot be instantiated

- *Deferred* binding:

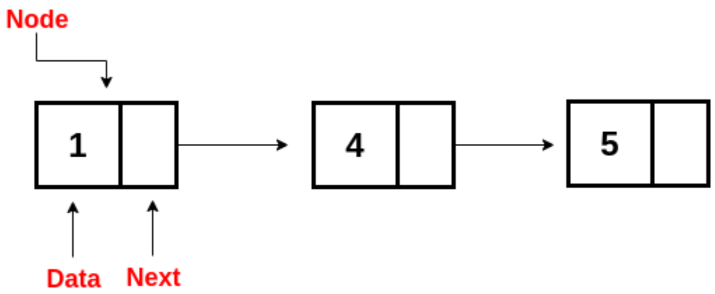
  not defined in the abstract type. Fixed interface for all the child classes → polymorphism

- *Non-overidable*:

  methods that cannot be overwritten by child types



Example: polymorphic linked list



Taken from src/basic/linked_list.F90

```
type :: linked_list_t
    private
    integer, public :: size = 0
    class(list_node_t), pointer :: first_node => null()
    class(list_node_t), pointer :: last_node => null()
  contains
    procedure :: add_node => linked_list_add_node
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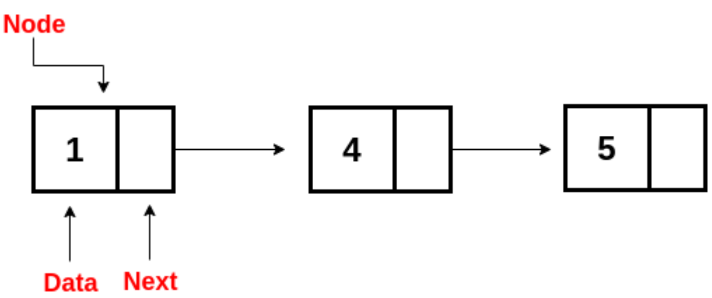

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The name of the class

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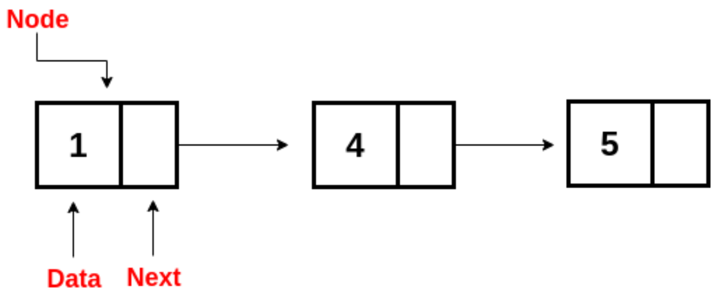


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By default, we want all attributes to be private

Good practice in general

Example: polymorphic linked list

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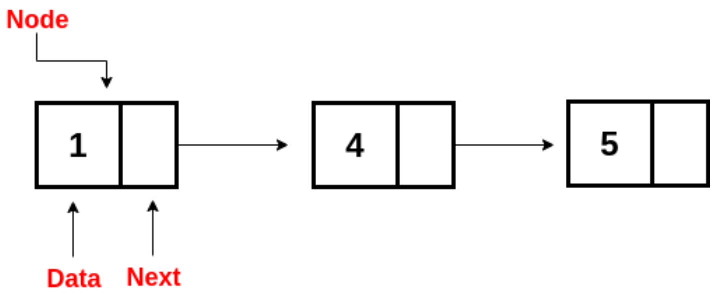


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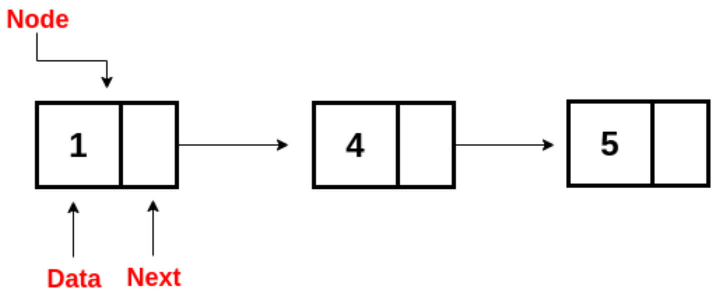
We want this attribute to be public

Example: polymorphic linked list



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```
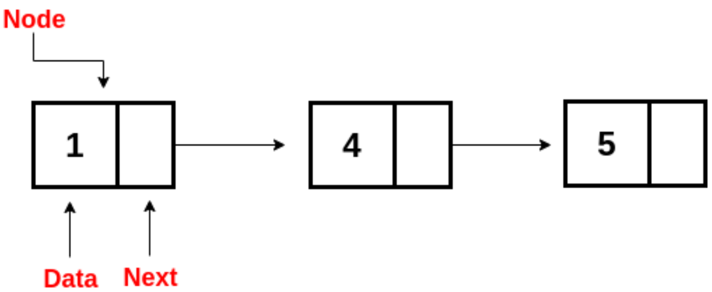

Pointer to a “class” *list_node_t*
This can also be any child class

Example: polymorphic linked list



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Type-bound procedures are defined below this point

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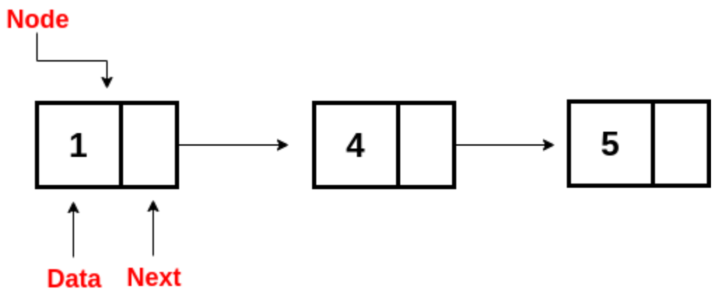


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```

Name visible for other objects
Can be identical for many classes

Actual name in the module
Needs to be different for each class

Example: polymorphic linked list

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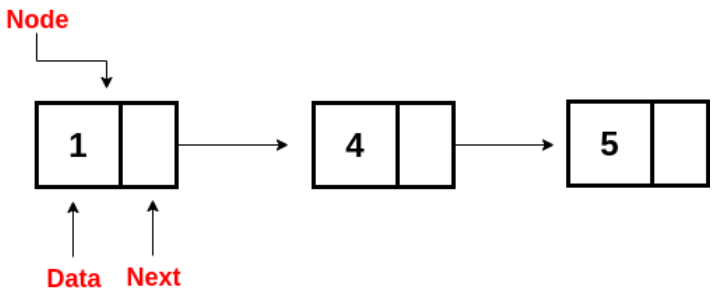


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  end type linked_list_t
```

Finalizer: a routine automatically called when the object is destroyed

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Example: polymorphic linked list

Taken from src/basic/list_node.F90

```
type :: list_node_t
  private
  logical :: clone
  class(*),          pointer :: value => null()
  type(list_node_t), pointer :: next_node => null()
contains
  procedure :: get => list_node_get
  procedure :: next => list_node_next
  procedure :: set_next => list_node_set_next
  procedure :: is_equal => list_node_is_equal
  procedure :: copy => list_node_copy
  final :: list_node_finalize
end type list_node_t
```

Example: polymorphic linked list

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 end type list_node_t
```

Points to any class: unlimited polymorphism

Together, we have a linked list of *list_node*, which are pointing to any possible class (*class(*)*)

Example: polymorphic linked list

Creating a child class: a list of integers

```
type, extends(linked_list_t) :: integer_list_t
   private
 contains
   procedure :: add => integer_list_add_node
 end type integer_list_t
```

Example: polymorphic linked list

Creating a child class: a list of integers

The class *integer_list_t* is a child of *linked_list_t*

```
type, extends(linked_list_t) :: integer_list_t
   private
 contains
   procedure :: add => integer_list_add_node
 end type integer_list_t
```

Example: polymorphic linked list

Creating a child class: a list of integers

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type, extends(linked_list_t) :: integer_list_t
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The class *integer_list_t* has a “add” routine

Example: polymorphic linked list

Creating a child class: a list of integers

```
type, extends(linked_list_t) :: integer_list_t
   private
 contains
   procedure :: add => integer_list_add_node
 end type integer_list_t


 subroutine integer_list_add_node(this, value)
   class(integer_list_t), intent(inout) :: this
   integer,               target        :: value

   call this%add_copy(value)

 end subroutine integer_list_add_node
```

The class *integer_list_t* has a “add” routine

We can only add integers using the add routine

Example: polymorphic linked list

Creating a child class: a list of integers

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   private
 contains
   procedure :: add => integer_list_add_node
 end type integer_list_t


 subroutine integer_list_add_node(this, value)
   class(integer_list_t), intent(inout) :: this
   integer,               target        :: value

   call this%add_copy(value)

 end subroutine integer_list_add_node
```

Here we call the routine of the parent class, which takes a class(*) argument
→ code reused !
→ abstraction
→ encapsulation
Only integers can be added. Avoids misuses of the list of integers.

Behind this line: 35 lines of fully generic code.

From the linked list to a time propagator

In essence, a time propagator is nothing but an algorithm, a list of operators

In Octopus, *propagor_t* extends *linked_list_t*

```
! ---------------------------------------------------------
 function propagator_verlet_constructor(dt) result(this)
   FLOAT,                       intent(in) :: dt
   type(propagator_verlet_t), pointer    :: this

   PUSH_SUB(propagator_verlet_constructor)

   SAFE_ALLOCATE(this)

   this%start_step = OP_VERLET_START
   this%final_step = OP_VERLET_FINISH

   call this%add_operation(OP_VERLET_UPDATE_POS)
   call this%add_operation(OP_UPDATE_INTERACTIONS)
   call this%add_operation(OP_VERLET_COMPUTE_ACC)
   call this%add_operation(OP_VERLET_COMPUTE_VEL)
   call this%add_operation(OP_FINISHED)

   ! Verlet has only one algorithmic step
   this%algo_steps = 1

   this%dt = dt

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We create the object here (← pointing to SAFE_ALLOCATE(this))

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Here we add elements to our list
These are "algorithmic steps"

From the linked list to a time propagator

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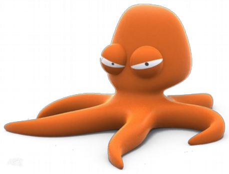
We can "read" the algorithm directly

Easier to debug !



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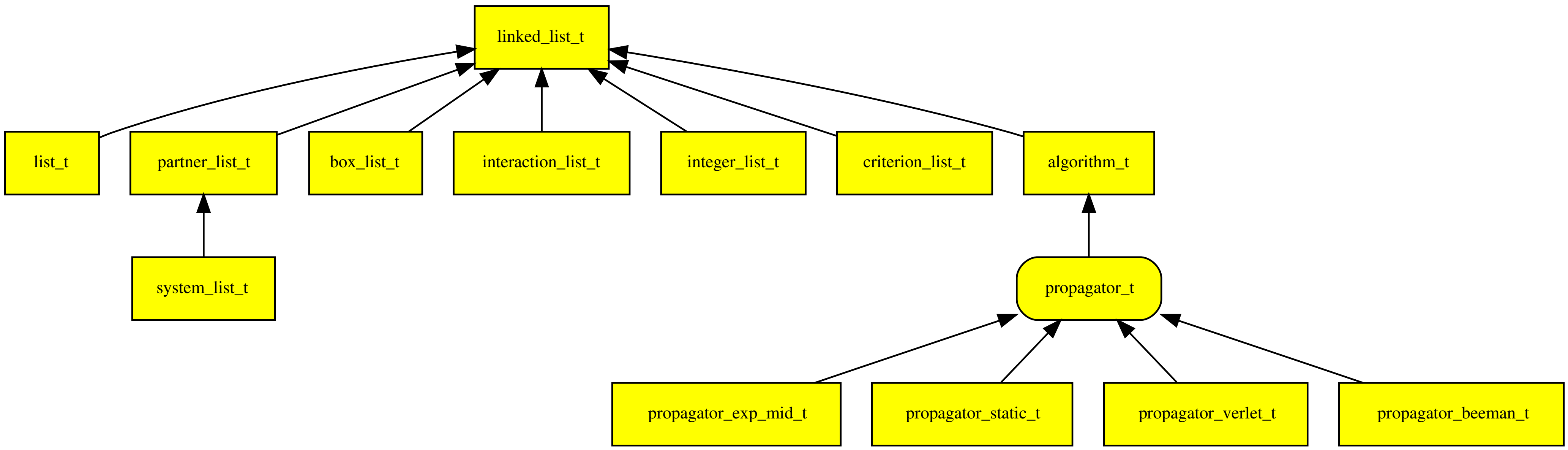
Some steps are generic
Code reusability

From the linked list to a time propagator



Knowing the type of an polymorphic object

Let’s come back to out list of integer

```
! ----------------------------------------------------------
  function integer_iterator_get_next(this) result(value)
    class(integer_iterator_t), intent(inout) :: this
    integer                                  :: value

    select type (ptr => this%get_next_ptr())
    type is (integer)
      value = ptr
    class default
      ASSERT(.false.)
    end select

  end function integer_iterator_get_next
```

Knowing the type of an polymorphic object

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get_next_ptr is a generic routine that returns a class(*) object...

Knowing the type of an polymorphic object

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Here we use *select type* to test the type of the object

Knowing the type of an polymorphic object

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      value = ptr
    class default
      ASSERT(.false.)
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  end function integer_iterator_get_next
```

Here we use *select type* to test the type of the object

Below this point, *ptr* is an integer