Octopus:
Coding paradigm

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Programming paradigms

Programming languages can be classified as:

- Imperative: instruct the machine how to change its state
  - Procedural: (old) Fortran, C, etc.
  - Object-oriented: C++, new Fortran, Python, Java, etc.
- Declarative: everything is defined as a function:
  given input leads to result. No side effects.
  - Functional: Mathematica, Lisp, etc.

Note: most programming languages do not exclusively fall into one category.

Procedual proramming

- based on procedure call
- procedures combine a series of computational steps
- can be called from everywhere in the program
- change the state of the computer (side effects)
- focus on variables, data structures and procedures
- usually, separation between data and procedures
- Examples: Fortran, ALGOL, COBOL, BASIC, C

Object Orientated Programming (OOP)

- focus on 'objects'
- objects contain the data and methods acting on them
- objects interact with other objects
- objects are instances of classes
- idea: hide internals of an object from the outside world
- Examples: C++, Java, Python, R, modern Fortran, ...

Object Orientated Programming (OOP) in a nutshell

class	'compound data type' with data specific methods
object	A concrete instance of an class that has properties and methods
encapsulation	Bundles data and methods that operate on the data, hiding internal complexities.
inheritance	Classes can be constructed from a parent, adding or modifying properties or methods
polymorphism	Ability of objects to take on different forms. Allows one interface to be used for a general class of actions.

Object Orientated Programming (OOP): Encapsulation

- Data and also methods can be 'private'
- Access through well defined interface
- Internals can be changed without affecting the rest of the code

Object Orientated Programming (OOP): Inheritance

- Derive new classes from existing ones, extending their functionality
- Example:
  - Parent: classical particle:
    - data: mass, position, velocity
    - methods: accelerate(Force, dt)
  - Child: charged classical particle: only add charge, keep the others

Object Orientated Programming (OOP): Polymorphism

- Same method can execute different behaviour
- Child classes can override methods of parent
- Routines/functions can accept parent or child classes as arguments
- Examples: Propagators
    - abstract propagator: defines method propagate(dt)
    - different implementations, derived from abstract propagator, e.g. `verlet`, `rk4`
    - `system` contains a propagator `prop`, can be instantiated as `verlet`, or `rk4`
    - some function of `system` calls: `prop->propagate(dt)`
    - this will work for all propagators defined for that system

Object oriented design (OOD) principles

- Object oriented programming allows for very structured code.
- Important to get the structure right
- Common design principles:

DRY	don’t repeat yourself avoid code duplication
KISS	keep it simple, stupid don’t make it more complicated than necessary
SOLID	five more detailed rules, see next slide.

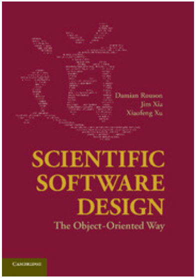
OOD: SOLID

- **Single responsibility principle (SRP):**
  A class should have only one responsibility.
  This makes the code easier to understand and maintain.
- **Open-closed principle (OCP):**
  A class should be open for extension but closed for modification.
  New features should be added to the class without modifying the existing code.
- **Liskov substitution principle (LSP):**
  Objects of a subclass should be substitutable for objects of their superclass.
  A subclass should be able to do everything that its superclass can do.
- **Interface segregation principle (ISP):**
  A client should not be forced to depend on methods that it does not use.
  A interfaces should be split into smaller, more specific interfaces.
- **Dependency inversion principle (DIP):**
  High-level modules should not depend on low-level modules. Instead, both should depend on abstractions.
  The code should depend on interfaces, not concrete implementations.

OOD: design patterns

For many situations, clear patterns have emerged.

- https://refactoring.guru:
  Overview of design patterns
- Scientific Software Design:
  The object oriented way
  (There is a copy in my office)



Object Orientation in Fortran

Some differences to 'proper' OOP languages (e.g. C++):

- no multiple inheritance
- less sophisticated polymorphism
- no templates! (that's a pain)

Some further reading:

- FortranWiki
- PGI introduction

Object Orientation in Fortran

- A `type` is a "class". It can be declared as abstract, or extend another `type`
- Polymorphism:
  - Declare an argument as `class(..)` instead of `type(...)`.
  - In order to access specific behaviour, we need a `select type` construct.
- *Abstract* type:
  can not be instantiated
- *Deferred* binding:
  not implemented in the abstract class; only define the interface for child classes
- *Non-overridable*:
  methods cannot be overloaded by child classes.

Object Orientation in Fortran: Example linked list

Example: linked_list.F90

- Definition of the class type `linked_list_t`
- Inheritance: `integer_linked_list_t`
- Unlimited polymorphism: `class(*)`
- `select type` construct:

Object Orientation in Fortran: Example linked list

```
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
  procedure :: add_ptr  => linked_list_add_node_ptr
  ...
  generic   :: assignment(=) => copy
  procedure :: empty => linked_list_empty
  final     :: linked_list_finalize
end type linked_list_t


type :: list_node_t
  private
  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
  final :: list_node_finalize
end type list_node_t

interface list_node_t
  procedure list_node_constructor
end interface list_node_t
```

- type bound methods
- overloading operators
- unlimited polymorphic pointer
- finalizer
- constructor

Object Orientation in Fortran: Example linked list

Example: linked_list.F90

- Inheritance: `integer_list`

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

- `select type` construct:

```
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
```

Object Orientation in Octopus

Where would we like to use OOP?

- Multisystem framework (more details later)
    - systems
    - interactions
    - propagators
- other 'objects':
    - Hamiltonians
    - operators (derivatives, ...)
    - grids, meshes
- low level objects:
    - mpi groups and communicators
    - linked lists
    - iterators
- This is work in progress...

Coding style

- Set of rules and guidelines for writing code
- Deals with indentation, white spaces, naming conventions, etc
- Makes the code easier to read and understand
- Ideally the code should read like plain English

Bad

```
if (space%periodic_dim > 0) then
  ...
end if
```

Good

```
if (space%is_periodic()) then
  ...
end if
```

- Helps avoiding some errors

Octopus coding standards

Some examples:

- Two space indentation
- No single letter variable names
- Module names end with `_oct_m`, derived types with `_t`
- All functions should go inside modules.
- All modules must have `private` and `implicit none` statements
- Intents for subroutine arguments are mandatory
- ...

`https://www.octopus-code.org/documentation/main/developers/coding_manual/coding_standards/`

Preprocessor

- Changes the source before compilation
- We use the C preprocessor:
  - Standard
  - Widely available
  - Requires some tricks to work with Fortran code
  - Imposes (few) limitations on Fortran code
- Several macros generated when running `configure` script
- Conditional compilation:

```
#ifdef HAVE_MPI
  ...
#else
  ...
#endif
```

- Templating to generate same subroutine with different data types (float/complex/integers, scalar/array, etc)

General code structure

- Use of macros and the preprocessor:
  - `#ifdef ... #endif`
    - conditional compilation
  - `SAFE_ALLOCATE()`
    - calls Fortran allocate()
    - returns error on failure
    - counts allocated memory for memory profiling
  - `PUSH_SUB() / POP_SUB()`
    - generates call stack for debugging
  - ”templating” (see later)
  - currently still many macros (e.g. types); most will be removed.

General code structure: Example

```
function energy_criterion_constructor(tol_abs, tol_rel, unit) &
                                     result(crit)

  FLOAT,                             intent(in) :: tol_abs
  FLOAT,                             intent(in) :: tol_rel
  type(unit_t),        target,       intent(in) :: unit
  class(energy_criterion_t),         pointer :: crit

  PUSH_SUB(energy_criterion_constructor)

  SAFE_ALLOCATE(crit)

  crit%tol_abs = tol_abs
  crit%tol_rel = tol_rel
  crit%unit => unit
  crit%label = 'energy'

  POP_SUB(energy_criterion_constructor)
end function energy_criterion_constructor
```

General code structure: "Templating"

- Some object oriented languages (e.g. C++) provide templates: code which is independent ot the data type
- Fortran does not provide templates
- Octopus uses macros as pseudo-templates:
  - macro `X(...)` prepends "type-prefix"
  - use macro `R_TYPE` as templated type in function definition.
- include functions as:

```
#include "undef.F90"
#include "real.F90"
#include "my_function_inc.F90"

#include "undef.F90"
#include "complex.F90"
#include "my_function_inc.F90"
...
```

Poor man's templates

- define functions as:

```
function X(my_function)(arg1, arg2) result(res))

  R_TYPE, intent(in)  :: arg1
  R_TYPE, intent(in)  :: arg2
  R_TYPE, intent(out) :: res
...
end function X(my_function)
```

- call functions as:

```
  real(real64)     :: da1, da2, dres
  complex(real64)  :: za1, za2, zres

  dres = dmy_function(da1, da2)
  zres = zmy_function(za1, za2)
```

General code structure: "Templating"

- If signatures differ, combine in interface

```
interface my_function
  dmy_function, zmy_function
end interface my_function
```

- We can't always do that.
  Examples: some batch functions
  (numerical type is hidden inside class)