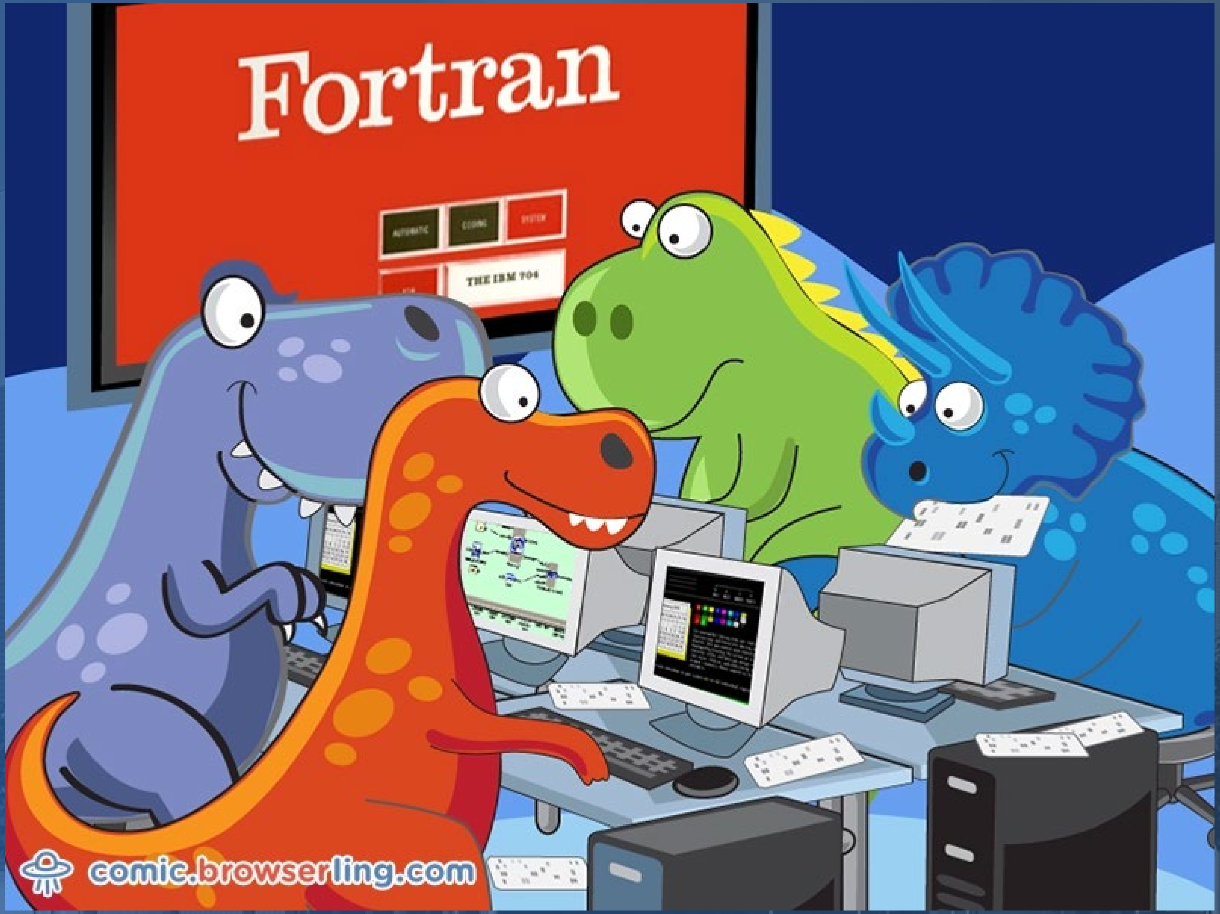
HPC Café

NHR@FAU – October 11, 2022

"Modern Fortran"

A contradiction in itself
or
A future-proof language?

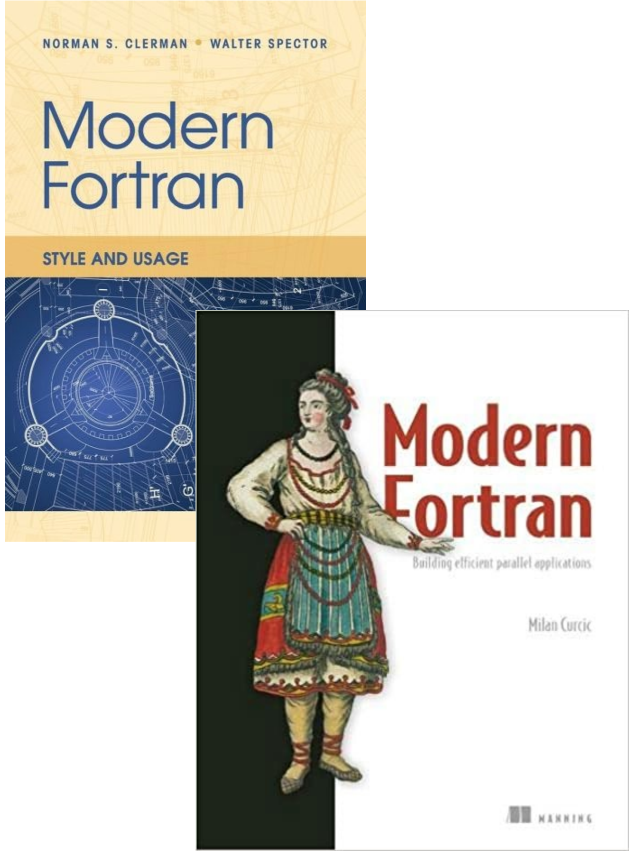


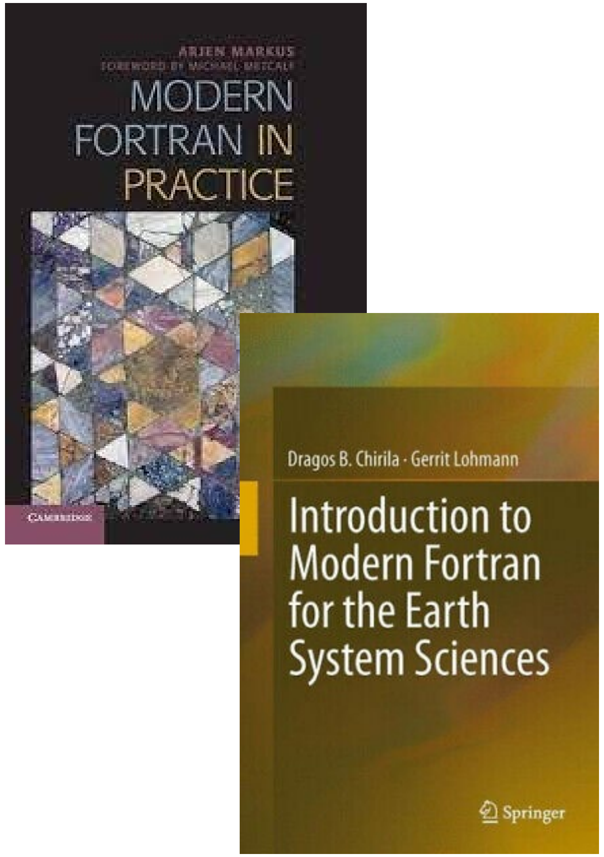
ISO-IEC 1539-1: Horses vs. Dinosaurs

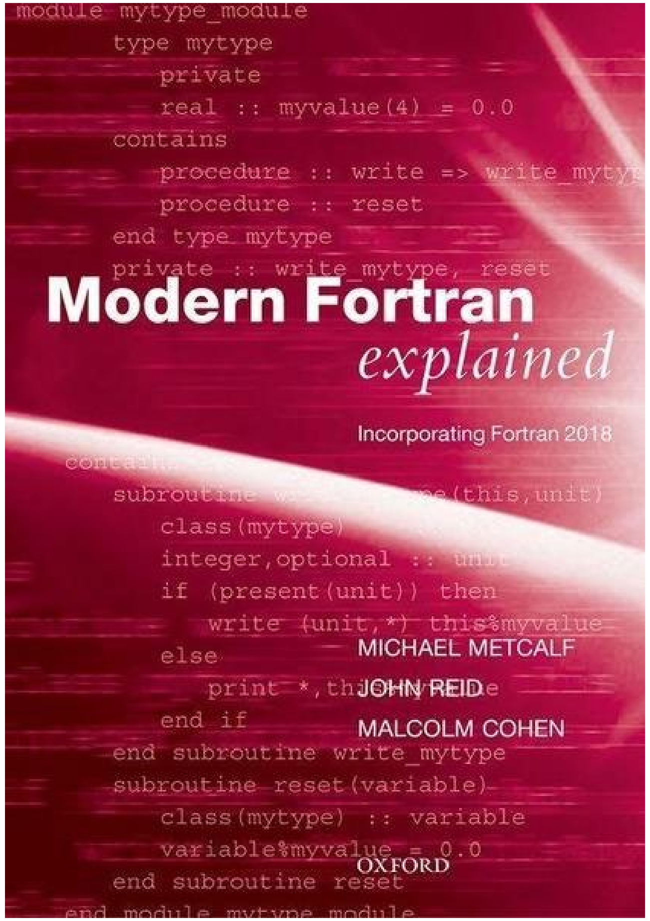
- this Dinosaur is in Use
  (... on both ends of the keyboard)
- Communities:
  Fortran is used for
  - data-intensive numerical calculations
    (need for optimization!)
  - nuclear weapons simulations
  - weather and climate modeling
  - quantum chemistry, biology
  - engineering (CFD, structural mechanics)
  - embedded components (R, python, ...)
- Learnability
  - good usefulness/effort ratio

- this Dinosaur has adapted
- Language evolution driven by
  ... **2** ... committees
  - feature definitions by
    ISO Fortran Language Committee
    („WG5“) https://wg5-fortran.org/
  - technical implementation by
    US National Body INCITS PL22.3
    („J3“) https://j3-fortran.org/

The Technical Literature does its best to keep up ...







What is "modern" about Fortran?

apart from cosmetic innovations ...

- Focus of FORTRAN 77
  - Portability
  - Performance

    (... for numerical algorithms)

- Focus today
  - Portability
  - Performance

    (... on scalable HPC systems)
  - Interoperability
  - Software Design and Engineering
  - Resiliency

    (... optional)

A la mode du jour ...

Fortran Standard

New Concepts in (and outside) Standard Generations

Fortran 90/95

- Module
  static Inheritance
  encapsulation
- Dynamic data
  Pointers
  allocatable Objects
- Type concept
  POD components
  dynamic components
- Array processing
- Parallelism ?
  FORALL — unimplementable
  OpenMP
  MPI (on crutches)

Fortran 2003

- Object orientation
  single dynamic inheritance
  type- and object-bound procedures
  abstract types and interfaces
- IEEE-754
- C-Interoperability
  C semantics in Fortran
- I/O extensions
  Asynchronous,
  Streams, UDDTIO
- Parallelism ??
  parameterized Data types
  (SoA vs AoS)
  OpenMP tasks

Fortran 2008

- Submodules
  Dependency inversion now for real !
- Parallelism !
  SPMD-PGAS:
  Coarrays

  DO CONCURRENT

  OpenMP simd
  OpenMP target

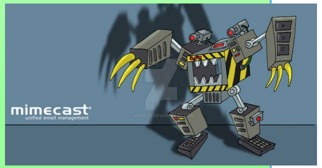
  MPI
  (still on crutches)

Fortran 2018

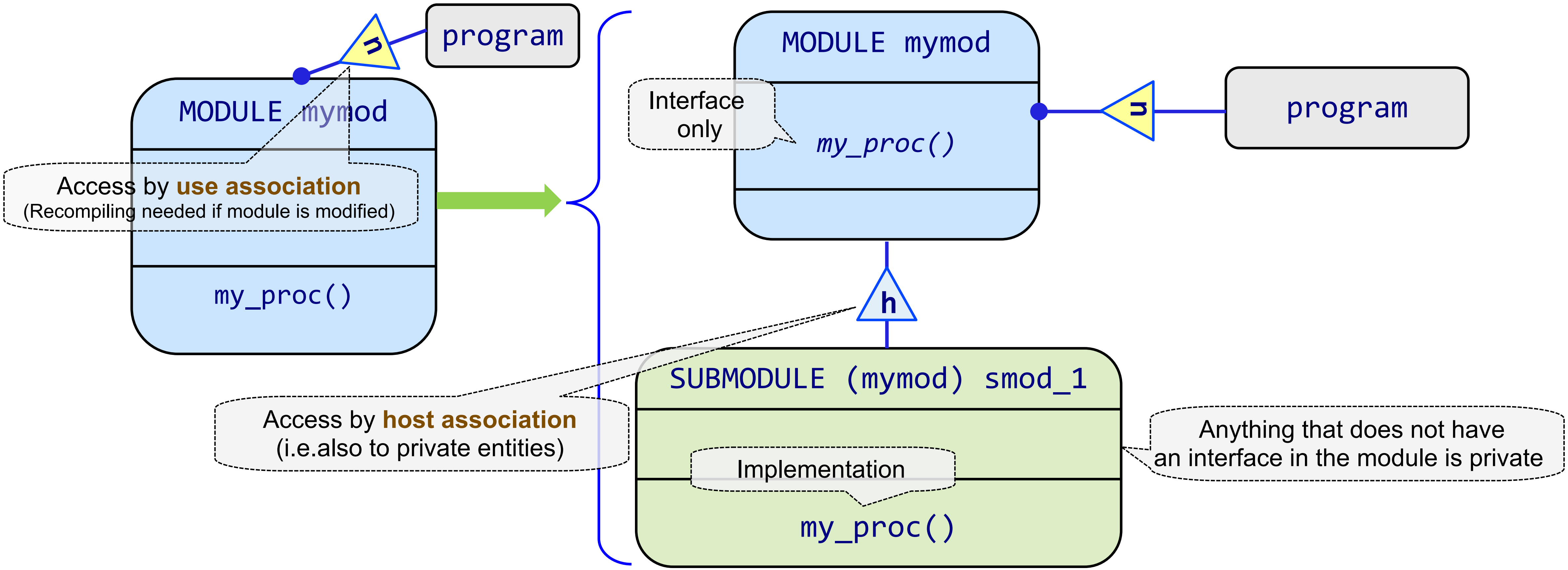
- C-Interoperability
  Fortran semantics in C
  Asynchronous extension
- Parallelism !!
  Coarray Teams
  collective intrinsics
  atomic intrinsics
  events

  DO CONCURRENT
  erweitert
  OpenMP

  MPI
  (nearly) without crutches!
- Resiliency
  optional



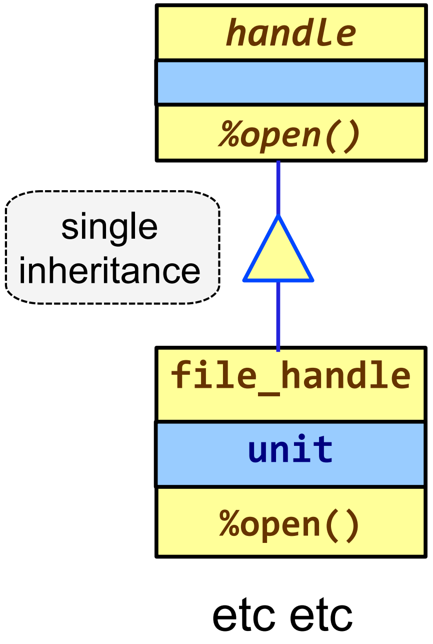
Dependency Inversion (1) – Submodules



- important modules are used by **many** other program units
  → "structural" Dependency Inversion
- deep submodule hierarchies are permitted, but likely of only limited usefulness

Dependency Inversion (2) – Interface class

- Abstract type and abstract interface




```
TYPE, ABSTRACT :: handle
CONTAINS
  PROCEDURE(open_handle), DEFERRED :: open
END TYPE HANDLE

ABSTRACT INTERFACE
  SUBROUTINE open_handle(this)
    IMPORT :: handle
    CLASS(handle) :: this
  END SUBROUTINE
END INTERFACE
```

```
TYPE, EXTENDS(handle) :: file_handle
    PRIVATE
    INTEGER :: unit
  CONTAINS
    PROCEDURE :: open => open_file_handle
  END TYPE file_handle
```

refers to an existing procedure

- Usage:

polymorphic (obligatory)

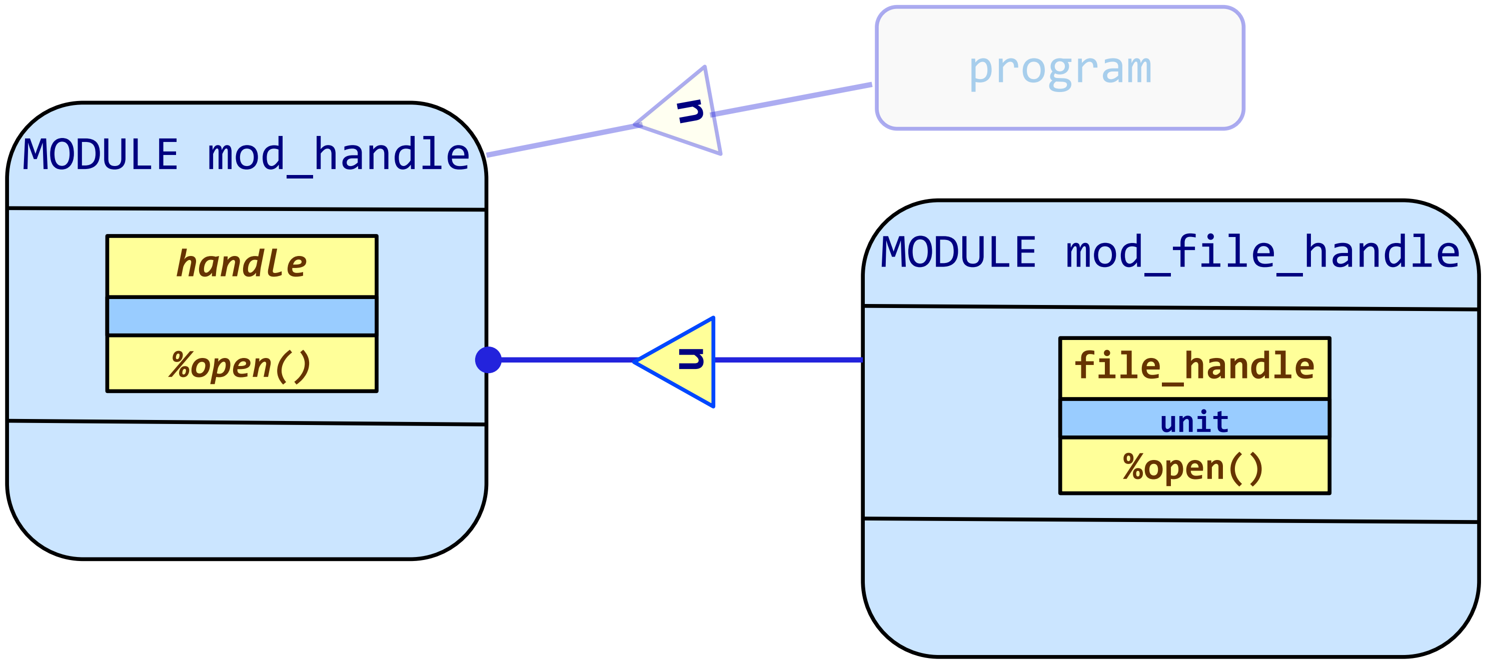
```
CLASS(handle), ALLOCATABLE :: my_handle

my_handle = ...

call my_handle%open()
```

auto-allocation

run time dispatch through a „virtual method"

- Observation: compile time access is only to abstract API
- „semantic" Dependency Inversion

Organisation of program units



- It would be nice if life were that easy ... but ...

What comes first – Hen or Egg?

- Creation of the polymorphic object ...

- **How?**
  - ➢ not possible through a method
  - ➢ ... since the latter needs the dynamic type of the object
  - ➢ which is in turn determined by the creation process.

- **Where?**
  - ➢ in the module that defines the abstract API
  - ➢ ... in order to preserve the structural Dependency Inversion

- Interface

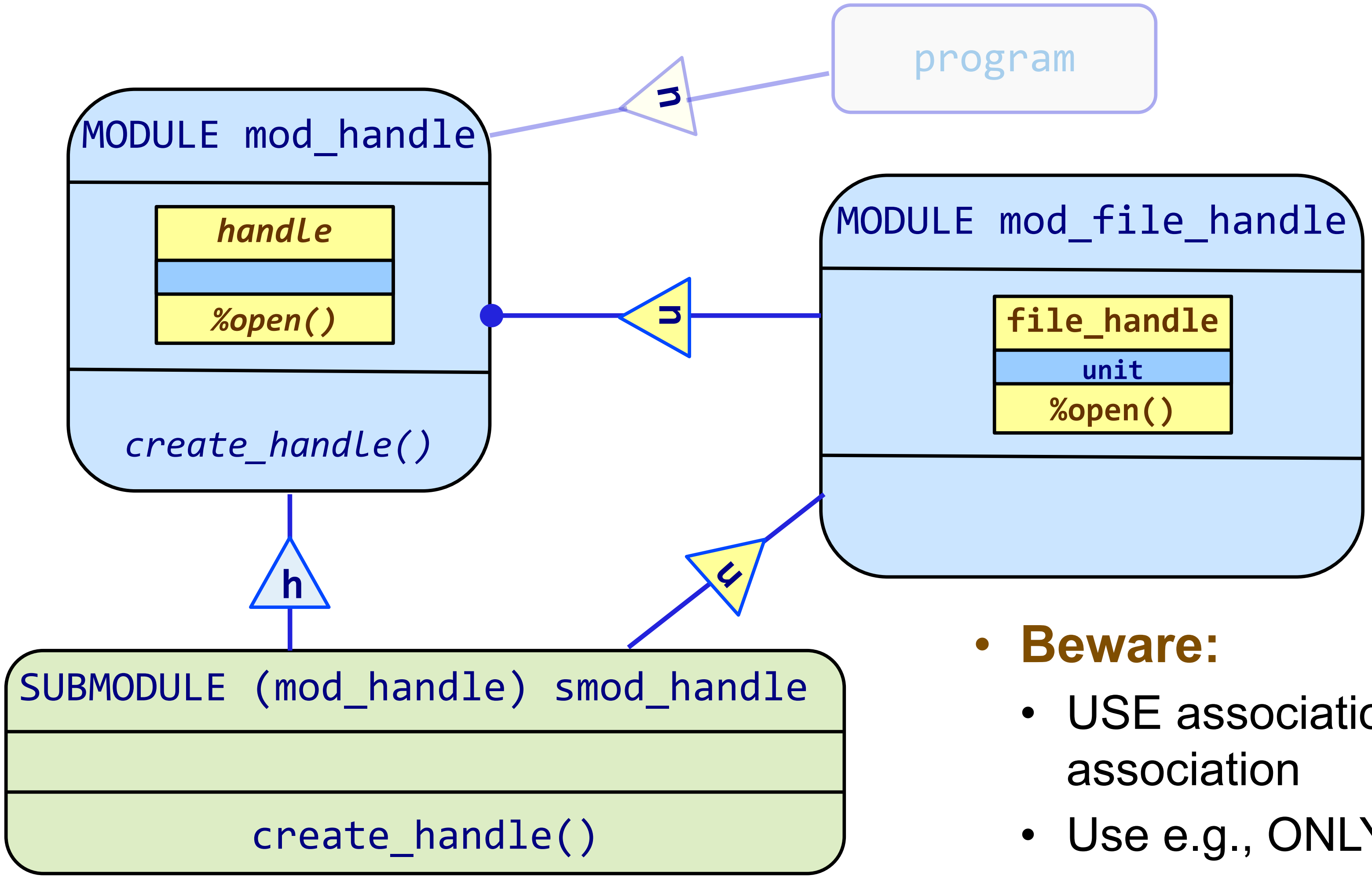
```
FUNCTION create_handle(htype) result(h)
  USE mod_file_handle, ONLY : file_handle
  CHARACTER(len=*), INTENT(in) :: htype
  CLASS(handle), ALLOCATABLE :: h
  ...
```

- Possible implementation

```
...
SELECT CASE(htype)
CASE 'file_handle'
  ALLOCATE( file_handle :: h )
  ...
CASE default
  STOP 'Unsupported extension of handle'
END SELECT
```

➢ USE access to definition of `file_handle` is needed → circular USE ⚡

Solution: combine structural and semantic Dependency Inversion



- **Beware:**
  - USE association overrides host association
  - Use e.g., ONLY to avoid side effects

Parallelism

- Within the Standard

  - Compiler-driven

```
DO CONCURRENT
   ...
END DO
```

independent iterations

    - additional clauses (locality, reductions)
    - hardware independent

  - Coarrays
    - Replication of serial program image (SPMD)
    - Scalable model

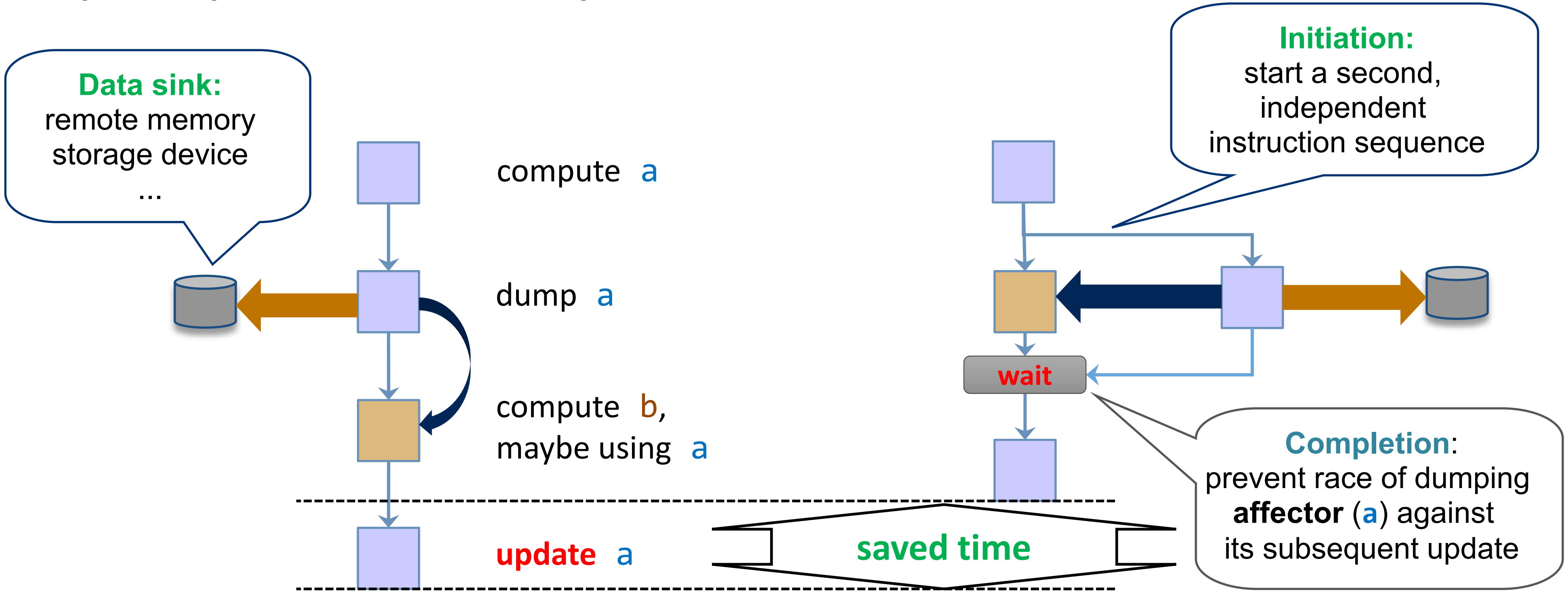
- Outwith the Standard

  - OpenMP - portable directives
    - Threaded execution in coherent shared memory
    - Vector units (simd)
    - Accelerators (offload)

  - Message Passing (MPI)
    - Replication of serial program image
    - Under control of communication library
    - Scalable model
    - **Standard conforming?**

Asynchronous processing

- overlap computation with independent data transfers



- Assumption:
  - ➢ additional system resources are available for processing the extra activity or even multiple activities (without incurring significant overhead)

Realization – non-blocking writes in MPI

- Specifications

```
USE mpi

REAL :: buf(NDIM)
INTEGER :: count, ierr, tag, req
INTEGER :: status(MPI_STATUS_SIZE)
```

- MPI rank 0

```
CALL mpi_isend(buf, count, MPI_REAL, &
               dest=1, tag, &
               MPI_COMM_WORLD, req, ierr)

:     Code that does not modify buf

CALL mpi_wait(req, status, ierr)
```

- Beware:
  - ➢ Implementation is not **obliged** to overlap communication and computation!

- MPI rank 1

```
CALL mpi_recv(buf, count, MPI_REAL, &
              source=0, tag, &
              MPI_COMM_WORLD, status, ierr)

:     Do anything with buf
```

Unfortunately, lots of bad things can happen ...

- Race conditions appear mysteriously (with a new and improved compiler and/or MPI library)

```
:
CALL mpi_wait(req, status, ierr)
buf = ...
```

optimizer's code motion

- Transmission of array section fails

```
CALL mpi_isend(buf(::stride), ...)
```

dummy argument is assumed size `DIMENSION (*)`, causing copy-in

- And, while we're at it,
  - none of the MPI calls with buffers are type-safe
  - reason: MPI buffers can be of **any type and rank**, but Fortran (up to 2008) lacks a concept for this
- So, apart from not really working, the MPI interface is not standard-conforming.
  - crutches: VOLATILE, MPI_F_SYNC_REG, directives for suppressing signature check

Resolution – use Fortran 2018 and the new MPI interface (> 3.1)

- Specifications

```
USE mpi_f08
REAL :: buf(NDIM)
INTEGER :: count, tag
TYPE(mpi_request) :: req
TYPE(mpi_status)  :: status
```

- MPI rank 0

```
BLOCK
  ASYNCHRONOUS :: buf
  CALL mpi_isend(buf, count, MPI_REAL, &
                 dest=1, tag, &
                 MPI_COMM_WORLD, req)

  :

  CALL mpi_wait(req, status, ierr)
END BLOCK
```

inhibits code motion (ASYNCHRONOUS :: buf)

Code that does **not** modify `buf` (:)

- `buf` dummy argument for `mpi_isend`

```
TYPE(*), ASYNCHRONOUS, INTENT(in) :: buf(..)
```

assumed-type (really the same as `*void`) — for `TYPE(*)`

assumed-rank — for `buf(..)`

- Array sections:

just to make sure

```
IF (MPI_SUBARRAYS_SUPPORTED) THEN
  CALL mpi_isend(buf(::stride), ...)
ELSE
  ...
END IF
```

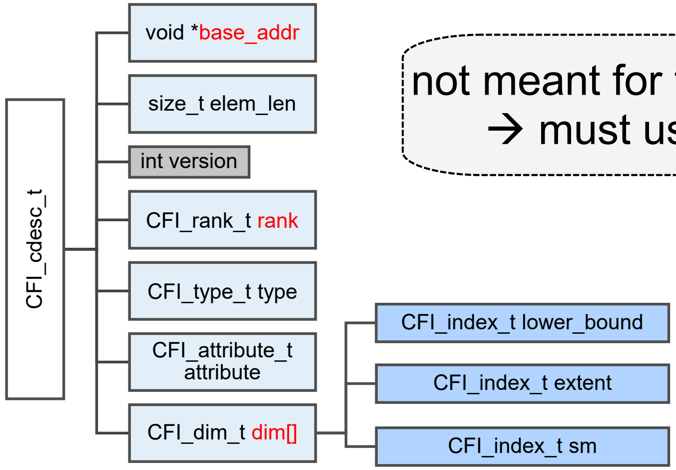
✓

The machinery behind assumed-rank ...

- Assume `mpi_isend()` has a BIND(C) interface:

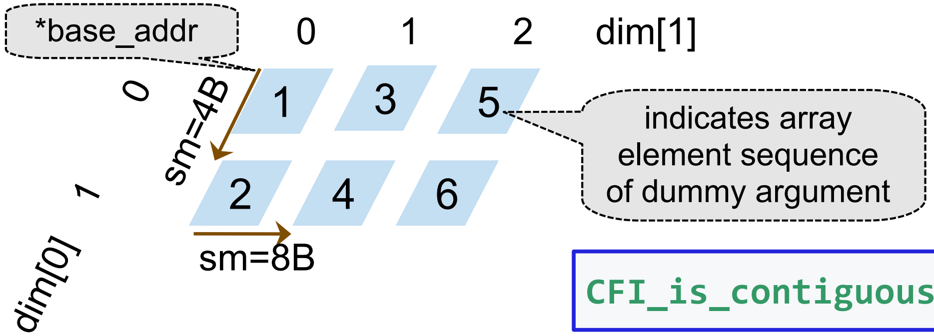
```c
#include <ISO_Fortran_binding.h>

void mpi_isend(CFI_cdesc_t *buf, ...);
```

- C descriptor for Fortran object



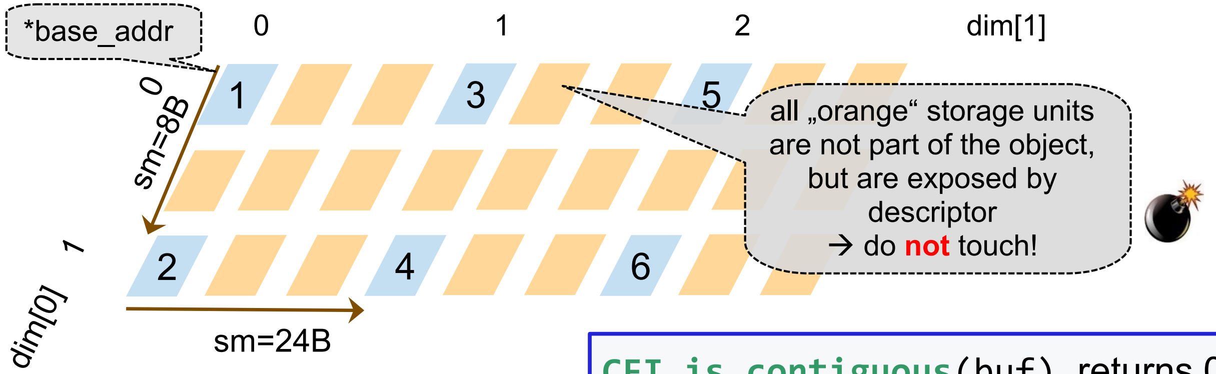
not meant for tampering
→ must use API

- Actual argument is a complete array (0:1,3)



`CFI_is_contiguous(buf)` returns 1

- Actual argument is an array section (0::2,1::3) of (0:2,9)



`CFI_is_contiguous(buf)` returns 0

Implement Fortran `mpi_isend()` in terms of C `MPI_Isend()`

Notional - I'm not saying it is done exactly this way ...

```
void mpi_isend( CFI_cdesc_t *buf, int count, MPI_Datatype datatype, int dest, int tag,
               MPI_Comm comm, MPI_Request *request, int *ierror ) {
   int ierror_local;
   MPI_Datatype disc_type;
   if ( CFI_is_contiguous( buf ) ) {
     ierror_local = MPI_Isend( buf->base_addr, count, datatype,
                    dest, tag, request, comm );
   } else {
     ...  /* use descriptor information to construct disc_type
             from datatype (e.g. via MPI_Type_create_subarray) */

     ierror_local = MPI_Isend( buf->base_addr, count, disc_type,
                    dest, tag, request, comm );
     ...  /* clean up disc_type */
   }
   if (ierror != NULL) *ierror = ierror_local;
}
```

C API always uses contiguous buffer

Using this was what you needed to do in "old" Fortran anyway ☹

PGAS Programming with coarrays (Fortran 2008)

- Asynchronous execution (SPMD)
  - **Images** `1, 2, …, num_images()`
  - each image has its own data

- Coarrays
  - Declaration with `CODIMENSION` attribute marks data as communicable

```
REAL :: a(ndim)[*]
REAL :: b(ndim)
```

(implicit) CODIMENSION attribute

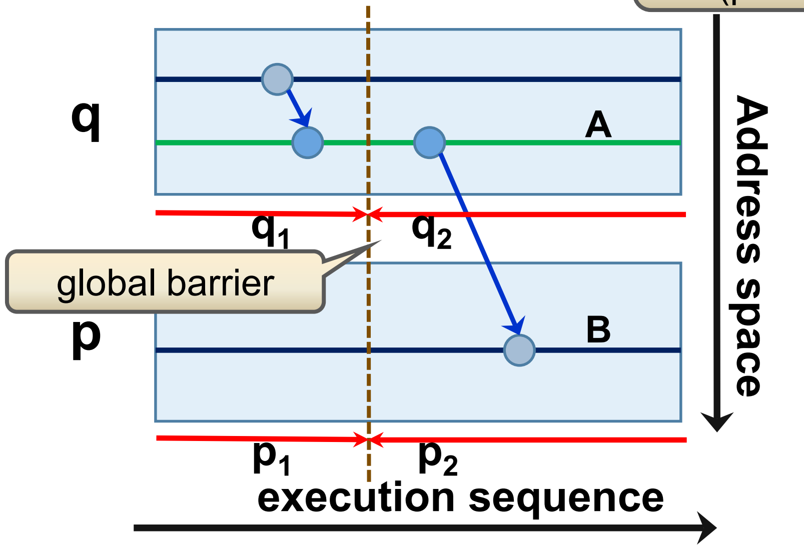
  - such data are **symmetric**: same type, rank and shape on all images
  - image-local accesses: as for non-communicable data

- Data transfer and synchronisation

```
a = …
SYNC ALL
IF (this_image() == p) &
      b = a(:)[q]
```

global barrier

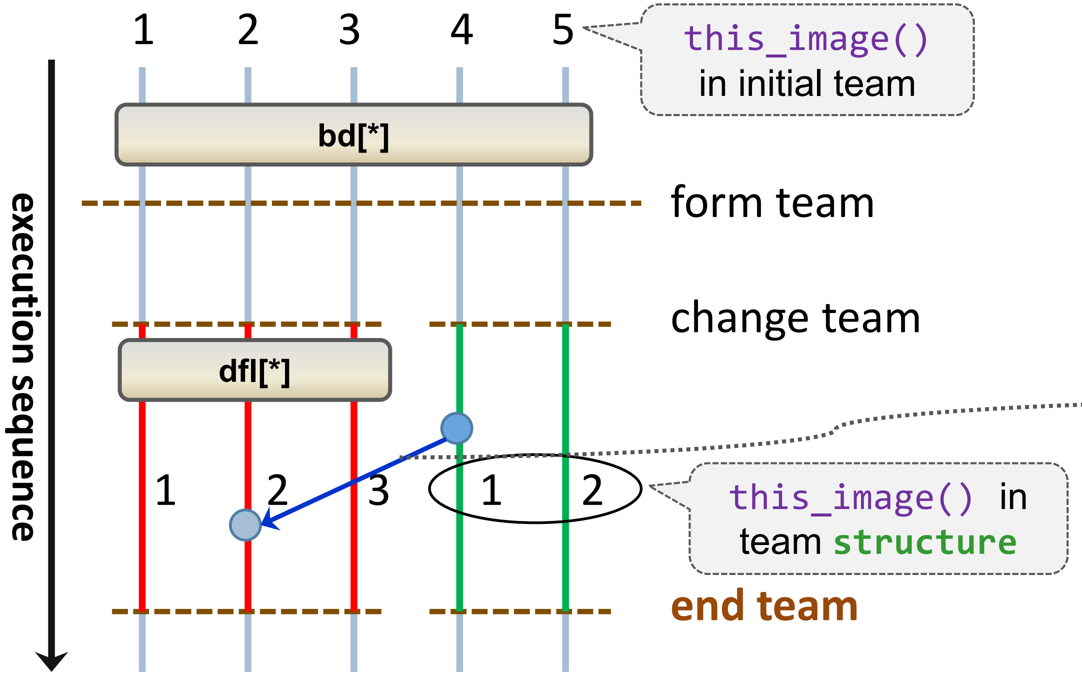
coindexed get (put also exists)



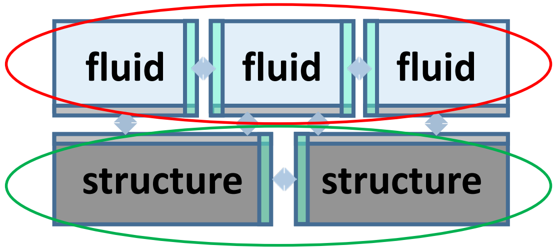
- Segment ordering:
  - **q_1 before p_2**, p_1 before q_2
  - q_j vs. p_j **unordered**

Coarray teams (Fortran 2018)

- Compose parallel programs



fluid und structure
are sibling teams



- Data exchange across team boundaries
  - is possible only for coarrays (`bd[*]`) that already exist prior to `change team` execution
  - the current team context must be preserved (no deallocation of `dfl[*]`) !
  - new syntax is therefore needed for coindexing, e.g.

```
… = bd(:,:)[ 4, TEAM=parent_team ]
```

  - cross-team synchronisation done with `sync team` (not shown here)

Usage scenarios for teams

- MPMD-style parallelism

- hybrid parallelism
  - team images within shared memory as potential optimization
  - recursive team decomposition (e.g. for „divide and conquer“ algorithms)

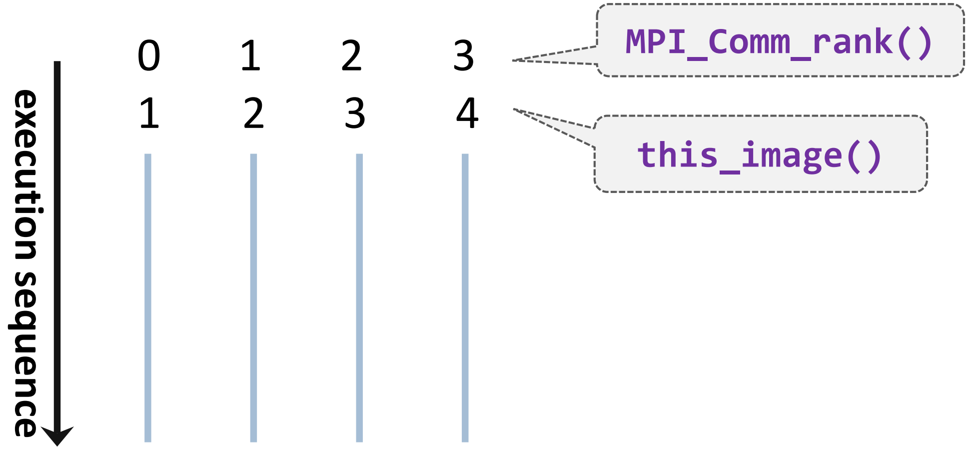
- Resiliency

  - optional feature: continue execution in the face of partial hardware failure (non-impacted images)
  - Defining a **spare image set** in a team decomposition allow the programmer to implement resilient applications
  - Requires significant programming effort to do properly, including reworking of parallel library components.

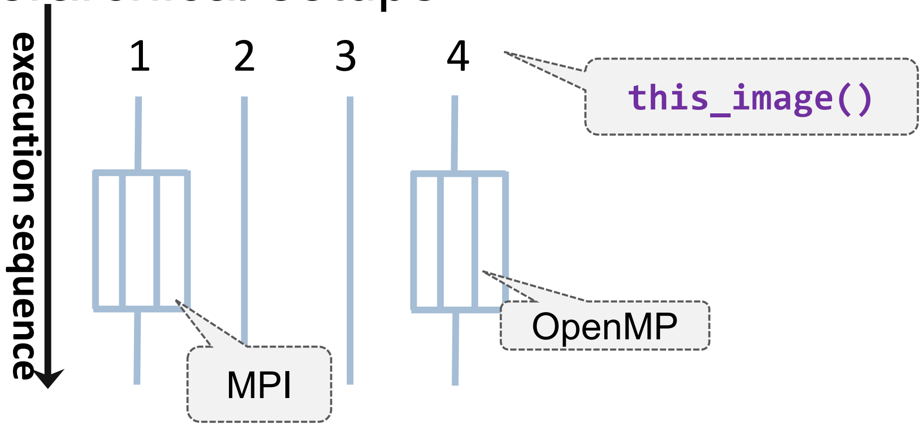
Combining parallel programming models?

- Yes, but ...
  - a multitude of design options (you need to decide on one early on)
  - high implementation dependency (portability suffers)
- MPI
  - MPI standard does not deal with coarrays and potential interactions
- OpenMP
  - currently no coarray support
  - separating to procedures should work
  - NAG does not permit this combination, however permits MPI „outside“ and coarrays „inside“

- MPI-coarrays one-to-one



- Hierarchical setups



Implementations
As of 2022

Compiler	Platform	Implementation	distributed memory?	Resiliency?
Intel Fortran („classic“)	x86	MPI based	yes	yes
GCC gfortran	multiple	MPI based (Opencoarrays)	yes	partial
GCC gfortran	multiple	shared memory, not all features	no	no
NAG Fortran	x86	shared memory (exclusive alternative to OpenMP)	no	yes (semantics)
Cray Fortran	Cray / HPE	low-level communication library	yes	yes

Especially MPI based implementations:
leave headroom for scalability and performance

Parameterized data types

a yet-hidden treasure of object based programming

- „Array of structures“
- „Structure of arrays“ (Fortran 2003)

```
type :: body
   character(len=4) :: units
   real :: mass
   real :: pos(3), vel(3)
end type body
```

```
type :: body_p( k, ntraj )
    integer, kind :: k = kind(1.0)
    integer, len :: ntraj = 1

    character(len=4) :: units
    real(kind=k) :: mass(ntraj)
    real(kind=k) :: pos(ntraj,3), vel(ntraj,3)
end type body_p
```

default values

produces desired representation

array dimension folded into component

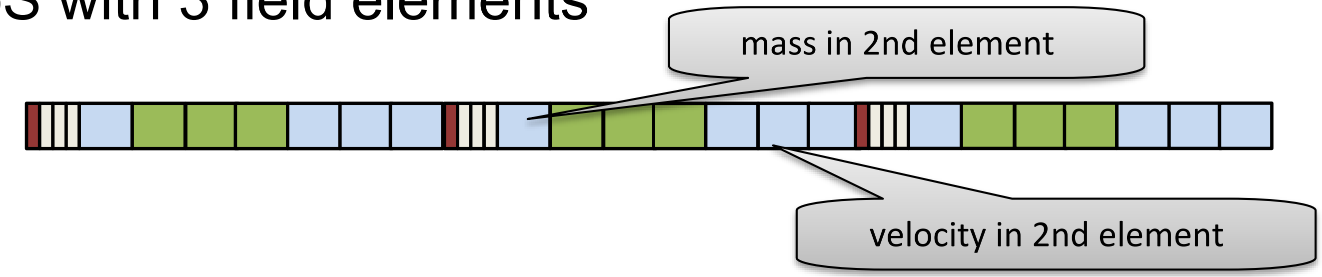
```
type(body), allocatable :: traj(:)
:
allocate( traj(3) )
```

```
type( body_p (ntraj=:) ), allocatable :: dyn_traj
:
allocate( body_p (ntraj=3) :: dyn_traj )
```

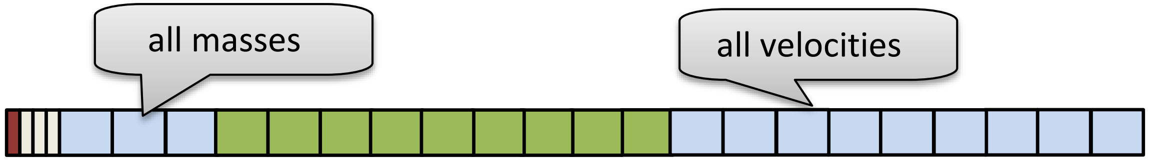
parameter belongs to type

Memory Layout

- AoS with 3 field elements



- SoA with LEN parameter value 3



actual memory layout
may differ in details

- AoS

  Memory accesses are typically non-contiguous

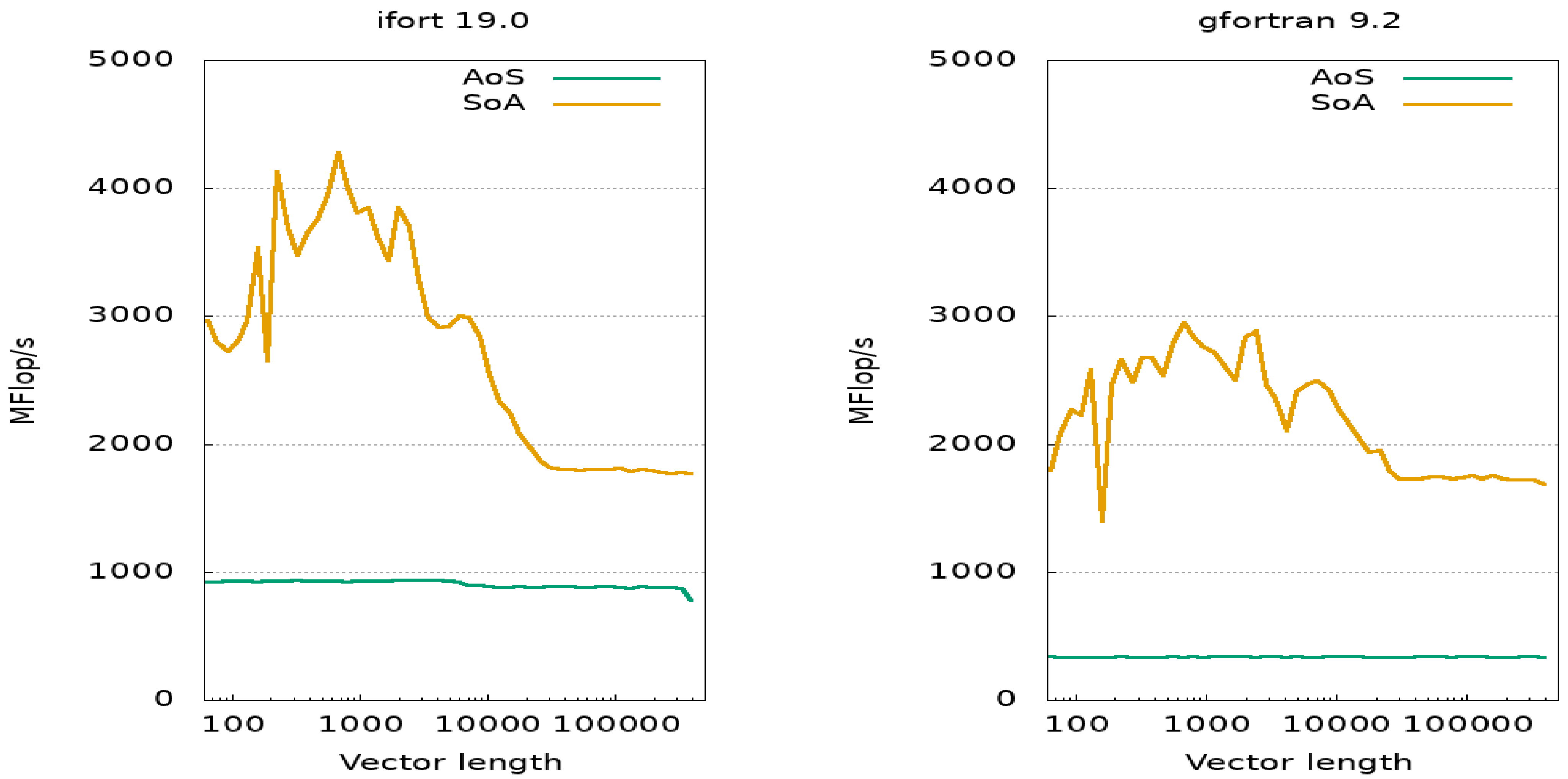
  → loss of „spatial locality“, independent of field size

- SoA

  supports contiguous access for all components

  → vectorizable
  → accelerators: efficient offload

Performance comparison for momentum transfer
(Intel Skylake 2.3 GHz)



Alternative: user allocatable components?

- Pro
  - Vectorization works
  - Implementations are mature
- Contra
  - Use as coarray is rather limited (avoid remote allocation)
  - Performance impact for data transfers through coarrays (additional latency for accessing unsymmetric memory)

Examle: scalar coarray of parameterized type

- symmetric memory!

```
type( body_p (ntraj=:) ), allocatable :: dyn_traj[:]
:
allocate( body_p (ntraj=256) :: dyn_traj[*] )
:
dyn_traj[p]%vel(:,:) = ...
sync all
```

update velocity data on remote image

⚠ Implementations are still immature

Fortran futures (1) – Fortran 2023

Currently in DIS stage

list is not complete

- Coarray extensions:
  - notify/wait mechanism for data transfer
  - arrays of a type with coarray components
- DO CONCURRENT:
  - REDUCE clause
- Declare object based on another object‘s type
  - TYPEOF / CLASSOF
- SIMPLE procedures
  - more restricted than PURE
  - PURE intrinsics are all SIMPLE
- Additional intrinsics (esp. for strings) and ISO_FORTRAN_ENV constants
- Extensions to array syntax
  - multi-subscripts, rank-agnostic DIMENSIONing
- Conditional expressions
  - both RHS expressions and actual arguments in procedure calls
- Enumeration types
  - both Fortran and C-compatible (more restricted), with slightly different syntax
- Additional edit descriptors
- Auto-allocation of error strings and internal records

Fortran futures (2) – Fortran 202Y

Already decided

- Templates (most likely) for generic programming
  - ➢ can be nested
  - ➢ parameters can be types, procedures ...
  - ➢ restrictions on parameters can be specified
  - ➢ no metaprogramming!
  - ➢ https://github.com/j3-fortran/generics/tree/main/examples

Feature is under active development

Potential further features

- Still under consideration!
  - ➢ extensions to collective intrinsics
  - ➢ extend data access to assumed-rank
  - ➢ ... many other small features

  - ➢ Current collection of requests (!) is at https://j3-fortran.org/doc/year/22/22-176r5.docx

Trying to answer the question from the cover page

- modern ... a contradiction in itself?

→No

✓ the language has been (and will be) re-honed to keep up with scientist‘s needs
✓ relevant software and engineering concepts have been added

❖ use best practices in new codes to avoid (problematic) legacy features

- ... future proof?

→Maybe

❖ performance portability is becoming more difficult to achieve
❖ insufficient support for accelerator hardware

„future“ is also a technical term:

```
future(id, device) : a = process(b, c)
:   ! do other stuff
wait(id)
```

fantasy syntax