

Computer Science in Ocean and Climate Research

Lecture 3: The Fortran Programming Language

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- 1 The Fortran Programming Language
 - Importance of Fortran for Climate Simulation
 - Fortran History
 - Different Source Code Formats
 - Some Special Features
 - Main Syntax Changes: Fortran 90
 - Compilation Process
 - Mixing Languages

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What is Fortran

- **Formula Translation**
- First higher programming language
- Originally procedural language
- Enhanced with object-oriented features
- Newest version: fully object-oriented

Tony Hoare, developer of Quicksort:

"I don't know what the language of the year 2000 will look like, but it will be called Fortran."

(Tony Hoare, taken from: Chivers, Sleightholme: Introduction to Programming with Fortran)

Why do we look at Fortran in this course

- Most climate models are written in Fortran...
- ...and also many simulations programs for technical and other scientific applications.
- Fortran Compiler is one of the top 10 algorithms of the 20th century (Society of Industrial and Applied Math. 2000)

from SIAM News, Volume 33, No. 4

The Best of the 20th Century: Editors Name to 10 Algorithms

by Barry A. Cipra

- For long time, Fortran was the language with the best compilers, i.e., the ones that generated the fastest code (then C became similarly fast).
- Many old codes (legacy codes) are written in Fortran. Often, a complete new implementation is too much effort.

Many numerically complex codes are still in Fortran

Standard Performance Evaluation Corporation

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CFP2006 (Floating Point Component of SPEC CPU2006):

Benchmark	Language	Application Area	Brief Description
410.bwaves	Fortran	Fluid Dynamics	Computes 3D transonic transient laminar viscous flow.
416.gamess	Fortran	Quantum Chemistry.	Gamess implements a wide range of quantum chemical computations. For the SPEC workload, self-consistent field calculations are performed using the Restricted Hartree Fock method, Restricted open-shell Hartree-Fock, and Multi-Configuration Self-Consistent Field
433.milc	C	Physics / Quantum Chromodynamics	A gauge field generating program for lattice gauge theory programs with dynamical quarks.
434.zeusmp	Fortran	Physics / CFD	ZEUS-MP is a computational fluid dynamics code developed at the Laboratory for Computational Astrophysics (NCSA, University of Illinois at Urbana-Champaign) for the simulation of astrophysical phenomena.
435.gromacs	C Fortran	Biochemistry / Molecular Dynamics	Molecular dynamics, i.e. simulate Newtonian equations of motion for hundreds to millions of particles. The test case simulates protein Lysozyme in a solution.
436.cactusADM	C Fortran	Physics / General Relativity	Solves the Einstein evolution equations using a staggered-leapfrog numerical method

437.leslie3d	Fortran	Fluid Dynamics	Computational (CFD) using Linear Algebra with the MacCormack time integrator
444.namd	C++	Biology / Molecular Dynamics	Simulates biological systems. Treats atoms of a molecule
447.dealII	C++	Finite Element Analysis	deal.II is a targeted at and error efficient solves a problem with non-linearities
450.soplex	C++	Linear Programming, Optimization	Solves a linear simplex algebraic planning problem
453.povray	C++	Image Ray-tracing	Image rendering 1280x1024 landscape objects with noise function
454.calculix	C Fortran	Structural Mechanics	Finite element nonlinear static Uses the Newton-Raphson method
459.GemsFDTD	Fortran	Computational Electromagnetics	Solves the wave equation using the finite domain (FDTD) method
465.tonto	Fortran	Quantum Chemistry	An open source package, designed in Fortran places a complex Hartree-Fock calculation experiment
470.lbm	C	Fluid Dynamics	Implement

How does a Fortran program look like

- Older programs are purely procedural
- Newer programs have object-oriented elements
- Because of the long history of the language there exist different standards ...
- ... and also different code formats (fixed, free format, s.u.)

For what purpose Fortran is useful?

- High Performance Computing (HPC)
- Computationally expensive numerical programs
- Simulations
- Many numerical libraries are written in Fortran
- Generally: everything that can be done also in C
- Coupling with C, C++, Java, Python is possible

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Fortran history

- Developed 1954-57 at IBM under John Backus (see Backus-Naur form, BNF, method to describe programming languages).
- Idea: enable programming of formulas in an effective way, without knowledge in hardware but also without performance losses.
- Proximity to hardware and efficiency more important than abstract concept.
- Replacement for Assembler programming for complex programs
- 1966: Standard Fortran 66 ASA (American Standards Association, predecessor of ANSI)



John Backus
1924-2007

Picture: Pierre Lescanne GNU FDL

Fortran history

from SIAM News, Volume 33, No. 4 (2000)

The Best of the 20th Century: Editors Name to 10 Algorithms

by Barry A. Cipra

- 1957: John Backus leads a team at IBM in developing the Fortran optimizing compiler. The creation of Fortran may rank as a single important event in the history of computer programming: Finally, scientists (and others) could tell the computer what they wanted it to do, without having to descend into the netherworld of machine code. Although modest by modern compiler standards - Fortran I consisted of a mere 23,500 assembly-language instructions - the early compiler was nonetheless capable of surprisingly sophisticated computations. As Backus himself recalls in a recent history of Fortran I, II and III, published in 1998 in the *IEEE Annals of the History of Computing*, the compiler "produced code of such efficiency that its output would startle the programmers who studied it."

Fortran versions

- 1957: Fortran I- IV, 1966: Fortran 66
- 1978: Fortran 77: still widely used, only fixed code format (fixed format)
- 1990: Fortran 90: New: free code format (free format), dynamic memory, advanced control structures (do-while), pointer, recursion, abstract data types, array operations ($A=B$). Some features of object orientation (modules containing data types and functions, similar to classes)
- 1996: Fortran 95: "cleaning", some redundant features are omitted, F95 compiler were faster.
- 2004: Fortran 2003: More object-oriented features (inheritance)
- 2010: Fortran 2008: Parallelization, coupling with C
- 2018: Fortran 2018: Smaller update

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- Fixed format (standard until F77): motivation by punch cards



Fixed format

Special meaning of columns:

- 1: commentary
- 2-5: labels
- 6: continuation mark
(concatenation of two lines)

```

Fortran - NSt_instantan/cgn.f - Eclipse SDK - /Users/ts/Documents

subroutine cgn(a,u,bb,scal,nmax,eps)
implicit none
include 'param.inc'
include 'num.inc'
include 'triang.inc'

real*8 a(ibp,nkpmax),scal(*),bb(nkpmax)
real*8 u(nkpmax),b(nkpmax),ha(nkpmax),d(nkpmax),r(n
real*8 delta,delta0,delta1,ddelta,alpha,beta,eps,r0
integer i,j,k,l,nmax

do i=1,nkp
  r(i)=r(i)-b(i)
  delta=delta+r(i)**2
  d(i)=r(i)
enddo

c Hirze
c
write(*,*) 'delta am Anfang cgn ', delta
close(4)
write(*,9998) tol,penf,penp,penu
format('tol=',e10.2,' penalty f=',e10.2, ' penalty p=',e10
' penalty u=',e10.2)
9998 *
c

```


Since Fortran 90: Free format

- Most of the restrictions of F77 are omitted
- Continuation mark now at the end of the line
- Commentary starting with "!" to the end of the line.

```
!
! bgc.f90
! tmmbgc
!
! Model for P04 (phosphate, y(:,0)) and DOP (dissolved organic phosphorus, y(:,1))
! - assuming ybgc is zero
! - conforms to BGC_1D_API
!
! Created by Jaroslaw Piwonski (CAU) on 10.02.10.
! Copyright 2010 CAU. All rights reserved.
!
subroutine bgc(t, dt, lat, insol, dayfrac, ice, wind, ntracer, nlayer, h, d, salt, 1
  implicit none
  ! input variables
  real*8 :: t, dt, lat, insol, dayfrac, ice, wind
  integer :: ntracer, nlayer, nparam
  real*8 :: h(0:nlayer-1), d(0:nlayer-1), salt(0:nlayer-1), temp(0:nlayer-1)
  real*8 :: y(0:nlayer-1, 0:ntracer-1)
  real*8 :: ybgc(0:nlayer-1, 0:ntracer-1)
  real*8 :: u(0:nparam-1)
  ! integer value parameters
  integer :: nbiostep = 8
  integer :: jeuphotic = 2
  ! real value parameters
  real*8 :: lambda ! remineralization rate : 1 /
  real*8 :: alpha ! maximum export rate : uM
  real*8 :: nu ! fraction of DOP
  real*8 :: K_P04 ! half saturation constant: P04 : uM
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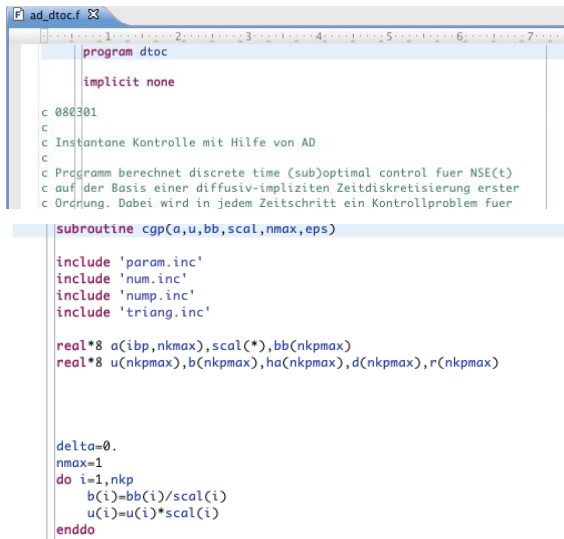
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Some special features of Fortran

- Case-insensitive
- Main program starts with keyword *program*
- Modularization: *subroutine*, *function*
- Data types: *integer*, *real*, *double precision* (*=real*8*)
- Arrays

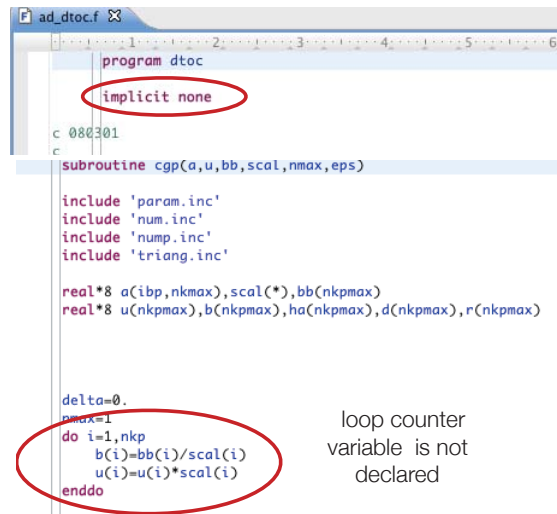


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```

Some special features of Fortran

- Implicit declaration of variables: variables that start with *i, j, k, l, m, n* are *integers*,
- ... others are *real*
- *implicit none* statement disables this feature and is recommended.
- Typical loop: *do ... enddo*



```
program dtoc
  implicit none

  c 080301
  c

  subroutine cgp(a,u,bb,scal,nmax,eps)

    include 'param.inc'
    include 'num.inc'
    include 'nump.inc'
    include 'triang.inc'

    real*8 a(ibp,nkmax),scal(*),bb(nkpmx)
    real*8 u(nkpmx),b(nkpmx),ha(nkpmx),d(nkpmx),r(nkpmx)

    delta=0.
    nmax=1
    do i=1,nkp
      b(i)=bb(i)/scal(i)
      u(i)=u(i)*scal(i)
    enddo
```

loop counter variable is not declared

end statement

- Old versions: no end statement for loops
- Jump labels and continues statement were used instead
- *continue* statement does not do anything
- ... was replaced by *enddo* statement

```
do 100 i=1,100  
c      do something  
100    continue
```

old: < F77

```
do i=1,100  
c      do something  
      enddo
```

new: since F77

Even worse ...

- Whitespaces in names are ignored
- Together with the implicit declaration and the usage of the *continue* statement (instead of an *end* statement) there could be problems.
- Left-hand picture: correct loop
- : Right-hand picture: typo: assignment to *real* variable *do100i* and no loop:

```
c      do 100 i=1,100  
      do something  
100    continue
```

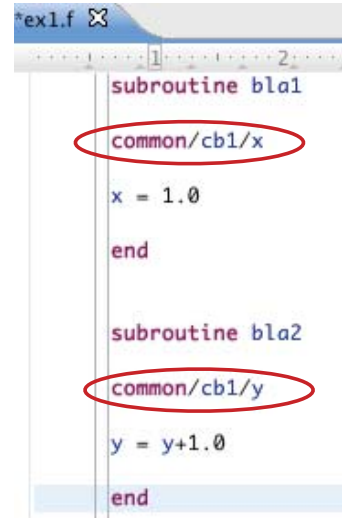
```
:      do 100 i=1.100  
      do something  
100    continue
```

- Famous Fortran bug that reportedly caused the crash of a rocket, but is now denoted as legend.

Some special features of Fortran

Global variables in *common* blocks:

- In every subprogram where the common block with the same name is used, the included variables are shared, ...
- ... even if they had different names in the respective subprograms.
- A common block represents a connected area of memory, having the length of the variables that are assigned to it,
- ... but types and names may be different in every subprogram, as long as the total memory in the common block remains the same.
- Error-prone!
- Can be found in many old programs.



The screenshot shows a code editor window titled '*ex1.f'. It contains two subroutines, 'bla1' and 'bla2'. Both subroutines use a common block named 'cb1'. In 'bla1', the common block contains variable 'x'. In 'bla2', the common block contains variable 'y'. The 'common/cb1/x' and 'common/cb1/y' lines are circled in red to highlight the shared common block.

```
*ex1.f
subroutine bla1
  common/cb1/x
  x = 1.0
end

subroutine bla2
  common/cb1/y
  y = y+1.0
end
```

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First improvements ... Fortran 90

- Modules instead of common blocks
- ... contain abstract data types and corresponding functions
- similar to C structs
- first step to object-orientation
- declarations with ::
- dynamically allocated memory: *allocate*, *deallocate*
- *do-while* loops

```
MODULE bla_module
  TYPE bla
    REAL :: x
    INTEGER :: y
  END TYPE bla

  CONTAINS

  SUBROUTINE blub
    ! do something...
  END SUBROUTINE blub

end bla_module
```

In F77: *gotos* and *arithmetic if*

Arithmetic IF

From Wikipedia, the free encyclopedia

The **arithmetic IF** statement has been for several decades a three-way arithmetic [conditional statement](#), starting from the very early version (1957) of [Fortran](#), and including FORTRAN IV, FORTRAN 66 and FORTRAN 77. Unlike the [logical IF statements](#) seen in other languages, the Fortran statement defines three different branches depending on whether the result of an expression was negative, zero, or positive, in said order, written as:

```
IF (expression) negative,zero,positive
```

While it was originally the only kind of IF statement provided in Fortran, the feature was used less and less frequently after the more powerful [logical IF statements](#) were introduced, and was finally labeled [obsolescent](#) in Fortran 90.

```
XES=0.0
XEC=0.0
DO 4 I=1,NEF
  ARG=BE(I)*T+CE(I)
  XES=XES+AE(I)*SIN(ARG)
  XEC=XEC+AE(I)*COS(ARG)
4 CONTINUE
ECC=SQRT(XES*XES+XEC*XEC)
TRA=ABS(XEC)
IF(TRA.LE.1.0E-08) GO TO 10
RP=ATAN(XES/XEC)
IF(XEC) 11,10,12
11 RP=RP+PI
GO TO 13
12 IF(XES) 14,13,13
14 RP=RP+2.0*PI
GO TO 13
10 IF(XES) 15,16,17
15 RP=1.5*PI
GO TO 13
16 RP=0.0
GO TO 13
17 RP=PI/2.0
13 PERH=RP/PIR
```

Fortran uses *call-by-reference* only ...

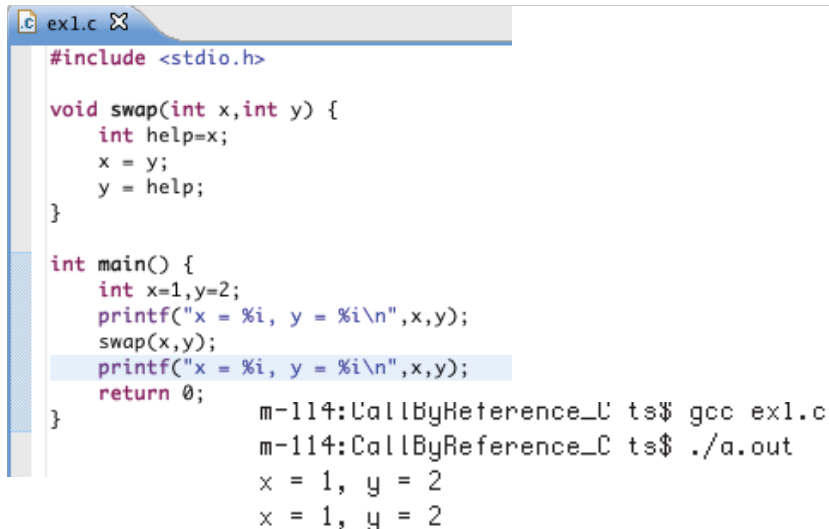
Exchange values of two variables

```
ex1.f90
1
2
3
4
5
program ex1
  implicit none
  integer :: x,y
  x = 1
  y = 2
  write(*,*) "vorher:  x= ", x, "y = ", y
  call swap(x,y)
  write(*,*) "nachher: x= ", x, "y = ", y
end program ex1

subroutine swap(x,y)
  integer :: x,y,help
  help = x
  x = y
  y = help
end subroutine swap
```

```
m-114:CallByReference ts$ gfortran ex1.f90
m-114:CallByReference ts$ ./a.out
vorher:  x=          1 y =          2
nachher: x=          2 y =          1
```

Different in C:



```
.c ex1.c X
#include <stdio.h>

void swap(int x,int y) {
    int help=x;
    x = y;
    y = help;
}

int main() {
    int x=1,y=2;
    printf("x = %i, y = %i\n",x,y);
    swap(x,y);
    printf("x = %i, y = %i\n",x,y);
    return 0;
}
```

m-114:CallByReference_C ts\$ gcc ex1.c
m-114:CallByReference_C ts\$./a.out
x = 1, y = 2
x = 1, y = 2

Fortran 90 and 95

- Array operations possible
- Similar to MATLAB[®]/Octave
- F95: additional *where* statement
- Built-in linear algebra routines (e.g., matrix multiplication).

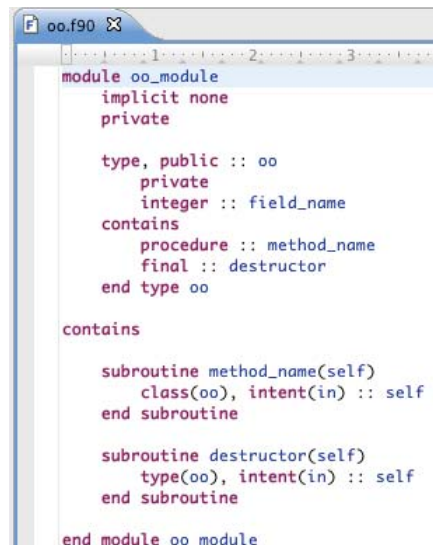
```
real :: A(10,10)
real :: B(10,10)

A = B
A = A + B

where (A < 0.0)
    A = 0.0
elsewhere
    ! ...
end
```

Fortran 2003/2008: Object-oriented programming

- Fortran class definition
- Defined in module
- Encapsulation (public, private)
- Element function/methods (keyword *contains*)
- Destructor (see C++, but not in Java)



```
oo.f90
1
2
3
module oo_module
  implicit none
  private

  type, public :: oo
    private
    integer :: field_name
  contains
    procedure :: method_name
    final :: destructor
  end type oo

contains

  subroutine method_name(self)
    class(oo), intent(in) :: self
  end subroutine

  subroutine destructor(self)
    type(oo), intent(in) :: self
  end subroutine

end module oo_module
```

Fortran 2003: Inheritance using submodules

Example (from ISO/IEC TR 19767)

<http://fortranwiki.org/fortran/show/Submodules>

```
module points
  type :: point
    real :: x, y
  end type point

  interface
    module function point_dist(a, b) result(distance)
      type(point), intent(in) :: a, b
      real :: distance
    end function point_dist
  end interface
end module points

submodule (points) points_a
contains
  module function point_dist(a, b) result(distance)
    type(point), intent(in) :: a, b
    real :: distance
    distance = sqrt((a%x - b%x)**2 + (a%y - b%y)**2)
  end function point_dist
end submodule points_a
```

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Fortran is a compiled language

Workflow:

- Write Source code → *file.f*
- Compile → generates *file.o* (*machine-dependent*)
- Link with library if necessary → executable
- Run executable

This means:

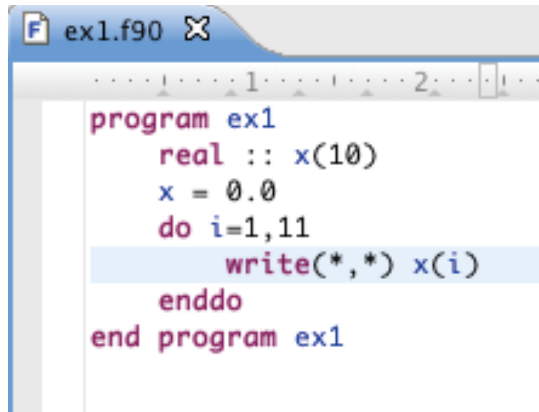
- Compiler is needed: *gfortran* gnu Fortran compiler, or *ifort*,...

Different compiler options for optimization, checking for syntax, floating-point exceptions

Fortran Compiler

- GNU (in gcc - gnu compiler collection):
 - older versions: g77,g95
 - now gfortran
- NAG (Numerical Algorithms Group)
- Intel (ifort), IBM (Name: *xlf*) own Fortran compiler
- more: Lahey, Portland (RZ-Cluster)

Fortran compiler allow many things



```
program ex1
  real :: x(10)
  x = 0.0
  do i=1,11
    write(*,*) x(i)
  enddo
end program ex1
```

```
m-114:ArrayTest ts$ gfortran ex1.f90
m-114:ArrayTest ts$ ./a.out
0.0000000
0.0000000
0.0000000
0.0000000
0.0000000
0.0000000
0.0000000
0.0000000
0.0000000
0.0000000
0.0000000
3.70672815E-38
```

Example: no check of array bounds

Contents

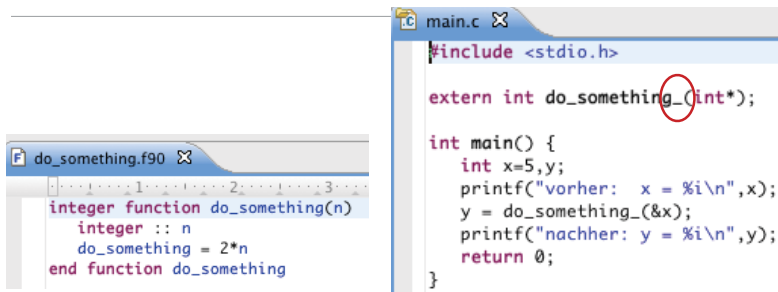
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Mixing languages

- Fortran subroutines and functions can be called from C and vice versa
- Compile source (e.g. with gcc and gfortran) and link object code with the same compiler
- Multi-dimensional arrays: Fortran stores column-wise, C row-wise
- Call-by-reference: always pass references/pointers from C to Fortran
- Java: JNI
- Python: F2py

Mixing languages: Some details may be important



The image shows two code editors side-by-side. The left editor, titled 'do_something.f90', contains Fortran code for a function. The right editor, titled 'main.c', contains C code for a main function that calls the Fortran function. In the C code, the parameter 'int' in the function signature 'extern int do_something_(int*);' is circled in red.

```
do_something.f90
integer function do_something(n)
  integer :: n
  do_something = 2*n
end function do_something

main.c
#include <stdio.h>

extern int do_something_(int*);

int main() {
  int x=5,y;
  printf("vorher: x = %i\n",x);
  y = do_something_(&x);
  printf("nachher: y = %i\n",y);
  return 0;
}
```

```
n-114:C_Fortran ts$ gfortran -c do_something.f90
n-114:C_Fortran ts$ gcc -c main.c
n-114:C_Fortran ts$ gcc main.o do_something.o -o a.out
n-114:C_Fortran ts$ ./a.out
vorher: x = 5
nachher: y = 10
```

What is important?

- Fortran was the first higher programming language.
- It was designed for and is well-suited for high performance programming.
- It is used in many applications.
- Especially in climate models, Fortran is the most important language.
- Fortran standards have developed in time.
- Most important standards are F77 and F90 and newer.
- Modern Fortran is fully object-oriented.
- Advanced array operations.
- Many climate models are legacy codes.
- Mixtures exist.
- Free and commercial Fortran compiler exist.
- Might be insensitive to bad programming habits (in standard settings).