IA! Modelling Tools Ma	ınual
	AHA! Modelling Tools Manual

# REVISION HISTORY

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#### Abstract

This document describes the modelling tools and approaches used for the new individual-based and agent-based model environment (framework). First, it documents the modelling **modules** that are developed to make coding such models simpler. Second, it outlines the general coding style and an aproach based on **object-oriented** programming.

Modern Fortran can be considered as an almost ideal language for agent-based modelling. It is high-level (e.g. it allows to work with whole arrays and slices) and partly object-oriented. It also contains many similar constructions with Python, so the later can be used for rapid prototyping. Nonetheless, it is compiled and strictly typed which makes coding big and complex projects safer. Compilers are easily available, including free GNU gfortran. Recent compilers generate highly efficient and extremely fast machine code. Modern Fortran includes some built-in parallel calculation instructions, and libraries and tools for high performance parallel computations are readily available. As such, Fortran is one of the favourite languages for computation-intensive works.

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SVN address of this document source is:

\$HeadURL: https://svn.uib.no/aha-fortran/branches/budaev/HEDTOOLS/BASE\_UTILS.adoc \$

Latest PDF version:

 $https://svn.uib.no/aha-fortran/trunk/HEDTOOLS/doc/BASE\_UTILS.pdf$ 

# 1 Software tools and requirements

Most tools needed for the model are already available on Linux (e.g. gfortran, make, Subversion, console, midnight commander etc) and are trivial to install using the standard package manager (e.g. apt-get install gfortran on Ubuntu). On Windows they can be installed manually from their official web sites. On Mac use homebrew to install many of the utils. Below are some details on the Windows software.

#### Fortran Compiler (Mandatory)

Intel Fortran compiler, a commercial software available at UiB. Intel Fortran is also installed on the UiB HPC cluster fimm. Free GNU Fortran distribution along with make and other tools is available from the Equation solution <a href="http://www.equation.com/servlet/equation.cmd?fa=fortran">http://www.equation.com/servlet/equation.cmd?fa=fortran</a>. There is also Oracle Solaris Studio combining Fortran compiler and an NetBeans-based IDE, freely available from <a href="http://www.oracle.com/technetwork/server-storage/solarisstudio">http://www.oracle.com/technetwork/server-storage/solarisstudio</a>, Linux and Solaris OSs only (no Windows or Mac).

#### **GNU Make** (Mandatory)

This is an automated program build system that keeps track of changes in different components of the source code and generates header files automatically depending on the platform and compiler used. It is possible to work without it, but in such a case everything should be tweaked manually. GNU make is trivial to install on Linux. For Windows, it goes bundled with the Equation solution GNU Fortran.

If GNU Fortran is not needed, make can be downloaded separately from the Equation solution web site.

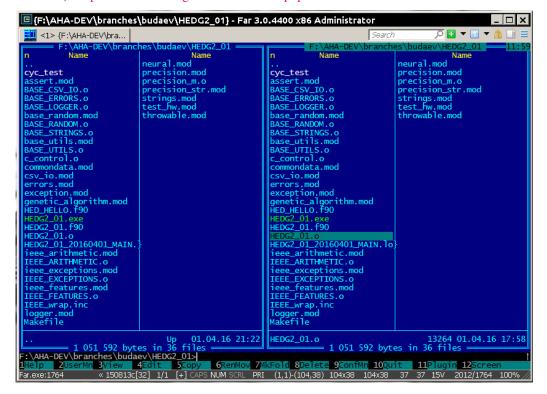
The official site of GNU make with the code, manuals etc. is here: https://www.gnu.org/software/make/

#### **Subversion** (Mandatory)

Windows GUI for Subversion is **TortoiseSVN** (supported by UiB IT): <a href="https://tortoisesvn.net/">https://tortoisesvn.net/</a>. It is very helpful to have also console Subversion client software: TortoiseSVN includes console tools but they are not installed by default. A good command-line-only Windows tool is SilkSVN <a href="https://sliksvn.com/download/">https://sliksvn.com/download/</a>. There are many other GUI tools, e.g. <a href="https://sliksvn.com/download/">PySVN-Workbench and TkCVS</a> that are open source tools available for Windows, Linux and Mac.

## Console terminal (Highly recommended)

The Windows console (cmd) is extremely weak. **Conemu** https://conemu.github.io/ is a much better alternative, especially with the **Far manager**, a two-panel console file manager similar to the ancient Norton commander for DOS (or Midnight commander on Linux): http://www.farmanager.com/download.php?l=en.



It is also very helpful to have (on the Microsoft Windows) the GNU core utilities (grep, cut, sed, awk etc.). Some of them are used in the GNU make build system, and some are included with the Equation solutions gfortran (TODO: have to check what is really necessary). There are several distributions available, e.g. GnuWin32, Cygwin, MinGW, UnxUtils, Gow, winbash.

#### **Doxygen: Automatically generate program documentation** (Highly Recommended)

This is a tool for writing software reference documentation. The documentation is written within code using special markup and can include formatting, formulas, tables, graphics etc. Doxygen can cross reference documentation and code, so that the user/reader of a document can easily refer to the actual code. It is trivial to install on Linux, but probably not so on Windows. Using the full power of the tool is not trivial though. Available from <a href="http://doxygen.org/">http://doxygen.org/</a>. On Windows is also highly desirable to have a LaTeX distribution, such as MikTeX (<a href="http://miktex.org">http://miktex.org</a>) and Ghostscript (<a href="http://www.ghostscript.com">http://www.ghostscript.com</a>), both are free software. LaTeX and Ghostscript are required to generate PDF.

#### Geany (Recommended)

Lightweight IDE, Editor for code and any text files (including AsciiDoc). Works on Linux, Windows and Mac. http://www.geany.org/Also need plugins: http://plugins.geany.org/ (The Geany SVN plugin for Windows *requires* command line tools like SilkSvn to work.)

## Code::Blocks for Fortran (Recommended)

IDE for Fortran. Works with many compilers, including Intel and GNU gfortran. http://cbfortran.sourceforge.net/. Installation by unpacking into some directory (i.e. does not require administrative rights).

#### Follow: A logfile reading program (Recommended)

Following a logfile while executing a program is done trivially on Linux: tail -f some\_log\_file.txt. There is a Java GUI program for reading log files that works on all major platforms installs by just placing in some directory: Follow. Available from http://sourceforge.net/projects/follow/.

# 2 Coding style: General guidelines and tips



### **Important**

A very helpful collection of advises and tips for efficient programming in Fortran can be found here: Fortran Best Practices

✓ **Avoid using very long lines of code.** They are difficult to read, especially if you (or your collaborator) use terminal editor limited by a 80 columns terminal. Working on the HPC cluster is always via the terminal. Also, compilers often do not like very long lines and may **drop extra characters** (resulting in compile errors). For example 132 characters is a standard limitation. But the default rules may be different on different compilers and platforms. Best try to use code lines limited by **80 characters** — many editors have options to show a 80-characters limit line at the right.



#### **Important**

In GNU gfortran compiler, <code>-ffree-line-length-N</code> flag controls how many characters (N) are allowed in a single line of code. The default value is 132. none removes any limnt, so the whole line is used: <code>gfortran -ffree-line-length-none</code> <code>code.f90</code>.

- ✓ Use the ampersand & line continuation symbol and indents to format code showing its structure for easy reading.
- ✓ **Avoid non-standard and non-portable Fortran constructions** that work on some compilers but not in others. Intel Fortran compiler can be especially notorious in implementing such constructs. Refer to the Fortran standard: Adams, J.C *et al.*, 2009. *The Fortran 2003 Handbook*. Springer, DOI: 10.1007/978-1-84628-746-6.
- ✓ Work at high level, use these tools, use objects, isolate as much as possible into subroutines In this way of coding, it becomes more clear what each part of the program is really doing and it is also easier to modify components of the program so that they don't affect other irrelevant components.

Modularise: many small subroutines are easier to code, test, understand, reuse, and maintain that a single monolithic piece or very few general subroutines. Modularity can also involve hierarchical organisation, it is sometimes quite useful, when a limited scope is required, to define subroutines within subroutines (the keyword contains can be used within other subroutines and functions!):

```
! This is the main module
module THE_GENOME
  use COMMONDATA
  implicit none
  . . . . .
  contains
  ! It contains this subroutine...
  subroutine chromosome_sort_rank_id(this)
   class(CHROMOSOME) :: this
    call qsort(this%allele)
    . . . . .
    contains
    ! And the above subroutine contains two further subroutines
    recursive subroutine qsort (A)
    . . . . .
    end subroutine qsort
    subroutine qs_partition_rank_id(A, marker)
    end subroutine qs_partition_rank_id
  end subroutine chromosome_sort_rank_id
end module THE_GENOME
```

✓ Use meaningful labels For example, using labels to mark do..end do, if ..end if, forall and other similar

constructs may greatly improve the readability of the code and make it more easy to understand, especially if there are many nested loops if..then..end if constructs. No need to label all such things (this will just increase clutter), but those that are really important or very big must be. A couple of examples are below:

```
SELECT_DEVIANT_CLASS: if (dev == 2) then
....
else if (dev == 3) then SELECT_DEVIANT_CLASS
....
else if (dev == 4) then SELECT_DEVIANT_CLASS
.....
end if SELECT_DEVIANT_CLASS
```

✓ Use whole-array operations and array slices instead of loops, prefer built-in loop-free and parallel instructions (where, forall etc.): it is faster. Fortran 95, 2003 and 2008 has several looping/array assignment constructions that have been optimised for speed in multi-processor parallel environments. Never use loops to initialise arrays, and avoid using them to calculate array components. Whenever possible, *reverse the order of indices* in nested loops, e.g. first looping should be over the columns, and then over the rows. Nested loops may have huge speed overhead! Use FORALL, WHERE and similar new "parallelized" Fortran constructions. Below is a little test conducted on an average amd64 system using GNU Fortran (-O3 -funroll-loops - fforce-addr, timing is by Linux time).

#### Test 1: Multiple nested loops, execution time = 0m12.488s

```
use BASE_UTILS
use BASE_RANDOM
implicit none
integer, parameter :: n=1000, a=100, b=100, c=100
integer :: nn, i,j,k
real :: random_r
real, dimension(a,b,c) :: M ! The above header part is the same in all tests
call random seed init
MATRLOOP: do nn=1, n
 random_r = rand_r4()
 do i=1, a
                                                      ! Multiple nested loops
   do j=1,b
      do k=1, c
       M(i,j,k) = random_r
      end do
    end do
  end do
end do MATRLOOP
```

#### Test 2: Direct array assignment, execution time = 0m1.046s

```
! header the same as above...
call random_seed_init

MATRLOOP: do nn=1,n
  random_r = rand_r4()
  M=random_r
end do MATRLOOP

! Direct array assignment
```

#### Test 3: forall instruction, execution time = 0m1.042s

```
! header the same as above...
call random_seed_init

MATRLOOP: do nn=1,n
  random_r = rand_r4()
  forall (i=1:a, j=1:b, k=1:c) M(i,j,k) = random_r ! Parallel instruction
end do MATRLOOP
```

### Test 4: Reverse order of nested loops (cols then rows), execution time = 0m1.046s

Multiple nested loops with the most "natural and intuitive" indices order (rows then cols) had a *really huge* execution speed overhead  $^1$ , more than *ten times* slower than the other methods (compare 12.5s and 1.0s!). The code is also more concise and easier to read. The same tests with Oracle Solaris Fortran (£95) turning on aggressive optimization and automatic loop parallelization (-fast -autopar -depend=yes) run much faster, but the speed differences still remained quite impressive (first test execution time = 0m0.010s, all other = 0m0.006s). So compiler-side aggressive CPU optimisation does work, although the tricks remain very useful.

Fortran has many built-in functions that work on **whole arrays** and these would be faster than multiple nested loops coded manually. For example, many arithmetic functions (abs, ... cos,... log, ... sin...) work with arrays as well as scalars. These are also useful: where, forall, as well as array logical operators with mask: all, any, count, maxloc, minloc, maxval, minval, merge, pack, unpack, product, sum. The code below illustrates some loop-free constructions:

```
! This program illustrates some loop-free Fortran constructions.
! Note that the order of indices here is: (column, row).
program LOOP_FREE
  ! Declare arrays and variables we need
 implicit none
 character(len=*), parameter :: fmt_str_r = "(3F8.1)" ! these are just for
 character(len=*), parameter :: fmt_str_i = "(318)"
                                                   ! output formatting
  ! Assign 2-D array values from a 1-D vector using 'reshape'
  real, dimension(3,4) :: A = reshape([1.1,2.1,3.1,&
                                        1.2 , 2.2 , 3.2 ,&
                                        1.3 , 2.3 , 3.3 ,&
                                        1.4 , 2.4 , 3.4 ] , [ 3 , 4 ] )
 integer, dimension(3,4) :: B = 0
 integer, dimension(3) :: S = 0
 logical, dimension(3) :: AB = F ! logical, can be either .TRUE. of .FALSE.
  ! Print original arrays
 print (fmt_str_r), A(:,1) ! 1.1 2.1 3.1
```

<sup>&</sup>lt;sup>1</sup> This is because allocation of arrays in the computer memory goes in an "index-reverse" order in Fortran, see http://www.fortran90.org/src/best-practices.html#multidimensional-arrays

```
print (fmt_str_r), A(:,2) !
 print (fmt_str_r), A(:,3) !
                                 1.3
                                         2.3
                                                 3.3
 print (fmt_str_r), A(:,4)
! *** Example 1: Assign values based on logical condition in 'where'
 where( A > 3.) ! 'where' clearly produces much simpler and
   A=100.
                           ! more concise code than two nested loops,
 elsewhere
                           ! it is also easier for the compiler to optimise
   B = 1.0
                           ! and therefore result in faster machine code.
 end where
  ! Here is the result of this array operation:
 print *, "----"
 print (fmt_str_r), A(:,1) ! 1.1
                                              100.0
 print (fmt_str_r), A(:,2) !
                                              100.0
                          !
 print (fmt_str_r), A(:,3)
                                 1.3
                                         2.3
                                              100.0
 print (fmt_str_r), A(:,4) !
                                         2.4
                                              100.0
 print *, "-----
                                 ______
 print (fmt_str_i), B(:,1) !
                                 1.0
                                         1.0
 print (fmt_str_i), B(:,2) !
                                  10
                                         1.0
                                                  0
 print (fmt_str_i), B(:,3) !
                                  10
                                         10
                                                  0
 print (fmt_str_i), B(:,4)
                          1.
                                  10
                                         10
! *** Example 2: Calculate sums of elements over the second (= rows) dimension
 S = sum(A, dim=2)
 print *, "-----
 print (fmt_str_i), S
                        1
                                                 400
! *** Example 3: Find if the condition holds, for all values over the second (rows)
               dimension, similar function 'any' evaluates for any of these values.
 AB = all(A > B, dim=2)! Here we output values .TRUE. as T or .FALSE. as F
                           ! F F T
 print *, AB
end program LOOP_FREE
```

Note that newer versions of Fortran compilers can become smart enough to adjust the order of looping in the machine code. Nonetheless it is better to write "optimised" code, preferably **not** requiring hand-optimisation of the looping order, such as **loop-free array constructions**, that works fast just everywhere. Many of the Fortran loop-free constructions actually resemble similar Matlab functions.

# 3 Document code as you write it with Doxygen

Doxygen is a very useful tool which allows to extract and produce documentation from the source code in a highly structured manner. Prior to parsing the code to get the documentation, one has to provide a configuration file for Doxygen. The doxywizard generates a wizard-like GUI to make this configuration file easily. There are many formatting symbols, Markdown codes are supported. Thus, it is easy to document the code extensively as it is being written.

Comments that are parsed through Doxygen are inserted into the source code using special markup language. The basic usage is quite simple. You should start comment line with "!>" rather than just "!", continuing Doxygen comments is done with two exclamation marks: "!!". Only comments formatted with this style are processed with Doxygen, you are free to insert "usual" comments, they are just ignored by the documentation generator.

The documentation description for a particular unit of the program, e.g. module, subroutine, function or variable definition, should normally go *before* this unit. Here is an example:

```
!! 'COMMONDATA' may also include subroutines/functions that have
general scope and used by many other modules of the model.
module COMMONDATA
.....
!> MODNAME always refers to the name of the current module for use by
!! the LOGGER function LOG_DBG. Note that in the debug mode (if IS_DEBUG=TRUE)
!! LOGGER should normally produce additional messages that are helpful for
!! debuging and locating possible sources of errors.
!! Each procedure should also have a similar private constant PROCNAME.
character (len=*), parameter, private :: MODNAME = "COMMONDATA"

!> This is the target string, only for the prototype test
character(len=*), parameter, public :: GA_TARGET = "This is a test of genetic algorithm."

!> Model name for tags, file names etc. Must be very short.
character (len=*), parameter, public :: MODEL_NAME = "HEDG2_01"
```

There are various options and keywords. A few of them should be particularly useful in documenting the model(s) codes:

@param describes a function or subroutine parameter, may optionally include [in] (or out or in,out) specifier. An example is below

```
subroutine LOG_DBG(message_string, procname, modname)
  implicit none
! Calling parameters:
!> @param[in] message_string String text for the log message
  character (len=*), intent(in) :: message_string
!> @param[in] procname Optional procedre name for debug messages
  character (len=*), optional, intent(in) :: procname
```

@returns describes a function return value. @retval is almost the same but starts with the function return value.

```
function TAG_MMDD() result (MMDD)
  implicit none
!> @retval MMDD Returns an 8-character string for YYYYMMDD
  character(8) MMDD
```

@brief starts a paragraph that serves as a brief description. @details starts the detailed description.

```
!-----
!> @brief LOG_DBG - debug message to the log
!! @details **PURPOSE:** This subroutine is a wrapper for writing debug
!! messages by the module 'LOGGER'. The debug message message
!! defined by the 'message_string' parameter is issued only
!! when the model runs in the debug mode, i.e. if 'IS_DEBUG=.TRUE.'
subroutine LOG_DBG(message_string, procname, modname)

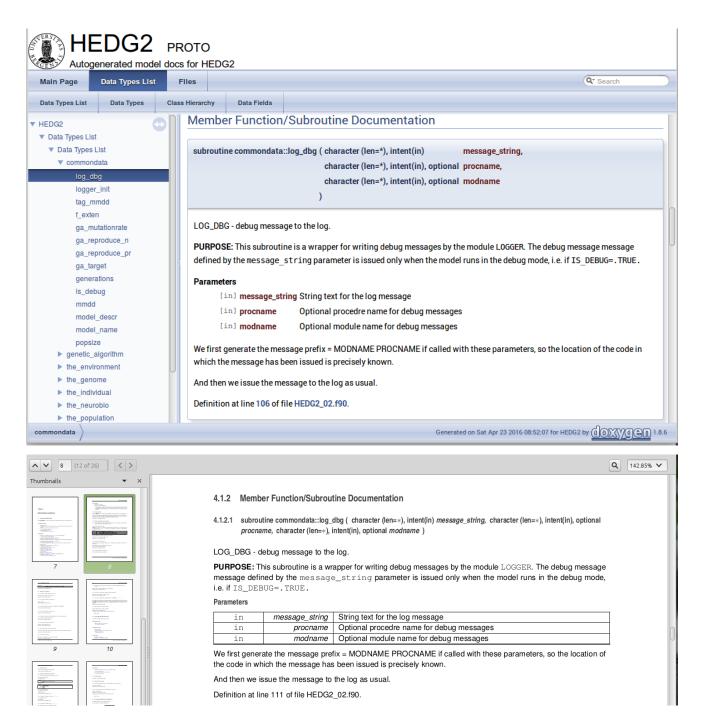
implicit none
```

@note insert a note with special emphasis in the doc text. @par start a new paragraph optionally with a title in parentheses. In the example above note also the use of **Markdown** formatting, such as double asterisks (\*) for strong emphasis (bold) and reverse quote (`) for inline code (variable names etc.).

Doxygen parses the source code and produces highly structured documentation in different formats (e.g. html, rtf, latex, pdf etc.).

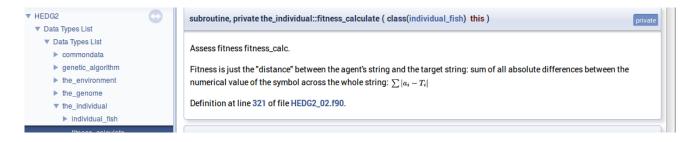
There are different options to generate HTML documents. For example, a bundle of HTML files with images, cross-references, code syntax highlighting and search functionality can be prepared. Alternatively, a single simpler HTML file can be done. LaTex output can be converted to PDF with references and index.

Examples of HTML and PDF outputs are below.



Here is an example of LaTeX formula in the autogenerated documentation file. Note that formulas are delimited with @f\$ on both sides.

This is rendered as follows:





#### **Important**

LaTeX, dvips and Ghostscript should be installed for the formula rendering to work correctly. There are webbased LaTeX equation editors, e.g. https://www.codecogs.com/latex/eqneditor.php

Documenting a complex model is very important! It is also not really difficult, but requires some additional discipline. It is much easier to include Doxygen comments as you write the model code than to look through the whole (huge) amount of the code a month later just to recall what the code is actually doing. Thus, the model becomes much more understandable to the level of its finest details. And Doxygen allows inclusion of various markup commands and styles, LaTeX formulas and graphics. Doxygen documentation, faq's and howtos are available here: http://doxygen.org

In the AHA GNU make system used to build the executables, documentation is generated using this simple command:

make docs

# 4 Version control: Subversion (SVN)

AHA Repository: https://svn.uib.no/aha-fortran

AHA Tools stable version (trunk): https://svn.uib.no/aha-fortran/trunk/HEDTOOLS/

Subversion (SVN) is a version control system used in the AHA project. Use version control not only for just managing versions, but also for organising your coding. For example, it would be good to commit changes to the server in pieces involving specific functions or parts of the model that are ready. Use the log messages to describe briefly what has been done. The examples below assume you use a terminal console, but most SVN commands can also be easily performed from a GUI tool.

For example, imagine you have implemented a new sigmoid function. Then, when it is ready, commit your change to the server with a log message like "New sigmoid function". And only after this go to the next piece of code. Then the versions you have will not be haphazard but organised into meaningful pieces. If you did several pieces in different files, e.g. sigmoid function in Hed18.f90 and a new Makefile for building the code, do two commits:

```
svn commit Hed18.f90 -m "New sigmoid function"
...
svn commit Makefile -m "Tweaked makefile, added PGI compiler build"
```

A typical SVN repository organisation usually includes a **trunk** directory for the main development line and many **branches** for different purposes created by different developers. For example, the current AHA repo has this structure:

```
|-- hormonemodel # One of the models, "production-ready"
'-- scripts # Templates of scripts and makefiles for reuse
```

The HEDTOOLS folder itself has the following structure

## 4.1 First time setup of the working copy



#### **Important**

AHA Tools in *trunk* (stable version) can be found here: https://svn.uib.no/aha-fortran/trunk/HEDTO OLS/; Development versions are here: https://svn.uib.no/aha-fortran/branches/budaev/HEDT OOLS/. So standard checkout (the *stable* version) is like this:

svn checkout https://svn.uib.no/aha-fortran/trunk/HEDTOOLS/

#### 4.1.1 Command line tool

First time setup of the working copy of the model (working directory):

• For a new project (run/experiment etc.), get into the working directory where the model code will reside (cd) (possibly make a new directory mkdir), and **checkout**: get the model code (one branch, no need to get everything!) from the server with svn checkout https://path\_to\_branch. When a specific repository is used *for the first time*, you should also include the user name for this repository (--username your\_user\_name) and then the program asks for the password. SVN server name, username and password is then saved, so subsequently it is not necessary to state the username/password you connect to the same SVN server from the same workstation. For example, first time checkout (for user u01):

svn --username u01 checkout https://svn.uib.no/aha-fortran/branches/budaev/HED18



next, just this should work:

```
svn checkout https://svn.uib.no/aha-fortran/branches/budaev/HED18
```

This will get the HED18 into the directory HED18 within the current working directory. If we use HEDTOOLS, it should also be placed here:

```
svn checkout https://svn.uib.no/aha-fortran/branches/budaev/HED18
...
svn checkout https://svn.uib.no/aha-fortran/branches/budaev/HEDTOOLS
```

So, we now get HED18 and HEDTOOLS in our working directory.

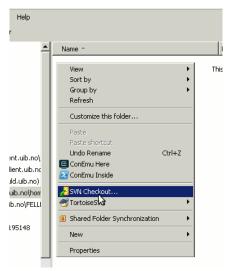
```
×
                         Terminal - sbudaev@fimm-1:~/work2
File Edit View Terminal Tabs Help
[sbudaev@fimm-1 work2]$
sbudaev@fimm-1 work2]$ svn checkout https://svn.uib.no/aha-fortran/branches/bud
aev/HED18
     HED18/Commonfish.txt
     HED18/NOTE.txt
     HED18/Hed18.f90
     HED18/RUN.pbs
     HED18/i101-parameters.txt
     HED18/Makefile
Checked out revision 506.
[sbudaev@fimm-1 work2]$ svn checkout https://svn.uib.no/aha-fortran/branches/bud
aev/HEDTOOLS
     HEDTOOLS/img_doc_fxce_svn.png
     HEDTOOLS/BASE_STRINGS.f90
HEDTOOLS/README_Notes.txt
     HEDTOOLS/BASE_UTILS.f90
     HEDTOOLS/.svnignore
     HEDTOOLS/BASE_UTILS.adoc
     HEDTOOLS/tests
     HEDTOOLS/tests/MODEL_PROTO.f90
     HEDTOOLS/tests/test_CSV_MAT.f90
     HEDTOOLS/tests/test_record_length.f90
     HEDTOOLS/tests/Makefile
HEDTOOLS/tests/test_CSV_IO.f90
     HEDTOOLS/BASE ERRORS.f90
```

#### 4.1.2 TortoiseSVN on Windows

• Using the TortoiseSVN on Windows, initial setup is also simple.

First, choose some folder for keeping the working copies of the development files, open it in the Windows Explorer.

Then right-click somewhere within this folder, then choose **TortoiseSVN** and click **Checkout**. This will bring a window to enter the Subversion repository address. Now paste the address of the folder you are going to clone on the local machine. It is perhaps good to get the HEDTOOLS modelling tools initially as they are used anyway.





## **Important**

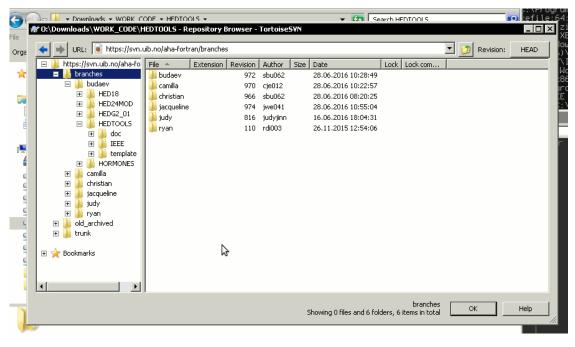
Unlike the command line client, TortoiseSVN by default clones to the repository directory into the current folder and **does not** create local folder with the same name as the remote one.

It may therefore be necessary to retype the *local directory name* the same as the remote one:

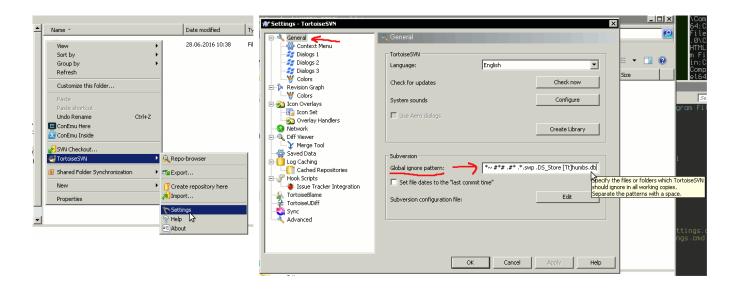


Initially the system will also ask for the username and password.

**Repository browser** that is called in the **Checkout** menu... button is a tool to explore the contents of the repository **on the server**. In **Checkout** menu it can be used to select the folder project to be cloned to the local machine. Also, using Repository browser you can make a private project directory on the server under /branches/your\_name and then clone it to the local system using the **Checkout** menu.



Alternatively, you can create project on the local machine first and use the menu item **Import** to import it to the repository. However, in the later case make sure you include only the Fortran (Matlab etc) **program code** into the Subversion and do not include the many accessory files created by the Microsoft Studio. They make clutter and are not needed in the versioning sytem. Use the **TortoiseSVN**  $\rightarrow$  **Settings**  $\rightarrow$  **Ignore** manu item for setting up ignore file patterns.



## 4.2 Standard workflow

Now you can work within this directory. This is the standard workflow.

- update code from the server: svn up
- edit the code using any favoured tools, build, run model etc...
- diff (svn diff) to check what are the differences between the local file(s) or directory and those in the repository, to use specific visual diff tool use --diff-cmd diff\_tool.
- commit when ready (e.g. when a new piece of code has been implemented): svn commit

commit will ask you to provide a short descriptive log message. It will run the standard text editor for this by default (can be configured). But you can provide such a message just on the command line with the -m option:

```
svn commit Hed18.f90 -m "New sigmoid function"
```

Both update and commit can be done for the working directory as well as for specific file. E.g. to commit only the model code Hedl8.f90 do:

```
svn commit Hed18.f90
```

Both update and commit can be performed within any subdirectory of the working copy. In such cases they are limited to this subdirectory only.

#### 4.3 Using branches

A **branch** in Subversion is just a directory on the SVN server. It can be thought of in the same way as common file system directory/folder. Creating a new folder is easy:

```
# Making a new directory for old code -- use the mkdir command
svn mkdir https://svn.uib.no/aha-fortran/old_archived
```

It is also easy to move or copy parts of the repository across the repository:

Do not forget to update the local working copy after deleting/moving/copying directories on the SVN server, then local copy will be in sync with the server.

#### 4.3.1 Make a branch copying old code

The copy command is very useful to create a copy of some repository part to a separate **branch**. Then some new features or functions can be implemented in the branch and then reintegrated back to the parent project. Or an independent new model can be initialised in such a way.

Making a branch is easy, use svn copy source\_svn\_path destination\_svn\_path to do this. For example, the following command makes a copy of the whole sub-tree for the model code HED18 from user budaev private branch to the user natasha private branch. Now natasha can work on her own copy of the code and, when done, merge the changes back to budaev's code. Finally, budaev's (and natasha's) code can be reintegrated back to the **trunk** main line.

```
svn copy https://svn.uib.no/aha-fortran/branches/budaev/HED18 \
   https://svn.uib.no/aha-fortran/branches/natasha/HED18 \
   -m "Creating private branch."
```

If several people are simultaneously working on the project, it make sense to merge changes from the parent branch back to the current branch (e.g. from trunk to budaev and natasha). Thus does not allow the code to diverge too far and reduces the chances to get version conflicts. Merging ongoing changes from the parent project is easy. For example, the following will merge changes from trunk back to the current branch (note that ^ substitutes the SVN repository web address):

```
svn merge ^/trunk/HEDTOOLS/
```

#### 4.3.2 Reintegrate your branch back to the trunk

Suppose you have a private branch/branches .../branches/budaev/HEDTOOLS where you work on the code. Now you are going to reintegrate your branch back to the trunk (the main development line: .../trunk/HEDTOOLS).

For this you need several simple steps:

**Step 1.** Merge possible changes in trunk back to the branch:

If someone is working on the trunk, you need to keep your branch in sync with it, e.g. all other files you are not working on are synchronised.

```
# First, make sure you are in the branch .../branches/budaev/HEDTOOLS
# Second, Do final check/update
svn status
svn update
# Merge possible changes from trunk to the (current) branch working copy
    --dry-run does everything but does not change any data, it is good to run it
    first to make sure everything is okay (e.g. yo are really in the correct
   directory, there are no errors etc.):
svn merge ^/trunk/HEDTOOLS/ --dry-run
# For example, if the working copy is not up to date (need commit or revert),
# there may be issues like this:
   svn: E195016: Cannot merge into a working copy that has local modifications
# to check what is wrong (modified), the command: svn diff is helpful. Also,
# commit local changes before merging.
# When everything is in order, do the real merge:
svn merge ^/trunk/HEDTOOLS/
# if merge was used, commit changes back to the repository, even though the
# files are unchanged, tags and properties may have changes
svn commit -m "Will merge back to trunk now"
```

Obviously, this first step is not always necessary. In many cases you can be sure that no one did changes in the trunk (or the other directoy to which merge is planned).

Step 2. Actually do the reintegrate changes from your branch back to the trunk. For this we need the code from the trunk.

```
# First, make sure you are in the trunk local working copy .../trunk/HEDTOOLS
# if necessary, checkout this directory somewhere just for this merge... but
# you need the code for the trunk.
pwd

# Second, do final checks/updates
svn status
svn update

# Do the reintegration of changes from branch back to (current) trunk working copy
# it is first good to try with --dry-run to make sure everything is okay
svn merge --reintegrate ^/branches/budaev/HEDTOOLS --dry-run
# and finally do the real thing
svn merge --reintegrate ^/branches/budaev/HEDTOOLS

# Finally, commit these changes back to the SVN repository
svn commit -m "Merged my changes to trunk"
```

## 4.4 Other features

Subversion has a very useful feature: you can set various properties (svn propset). For example, one can set tags on files or directories. A very interesting feature is that svn:keyword properties can be incorporated into the source files under SVN control. For example, you can include specific tags into the Fortran (or any other managed) source code so that they are updated automatically.

One user case for this is this. Define special \$Id tag. This tag includes the file name, last changed revision number, revision date and time and the user who did the revision. This is how it will appear in the source code:

```
! The comment below incorporates SVN revision ID, it should apparently be
! inserted into a comment, so does not affect the compiler:
! $Id: BASE_UTILS.adoc 1024 2016-06-29 14:21:11Z sbu062 $
! other code follows...
implicit none
.....
! Public constants
integer, public, parameter :: MAX_UNIT=255 ! Maximum unit number (in old
```

To set up this tag we just have to issue such command:

```
svn propset svn:keywords "Id" file_name_to_set_keyword.f90
```

and include two strings \$Id anything in between initially \$ in this source text to set where the keywords should be placed. Obviously, we have to **commit** change to the server after this. From now on, the information will be updated automatically between the \$id ... and \$ symbols. So the source code itself will have comments indicating the revision number etc. There are many useful tags that can be placed in such a way. For example \$Date \$Revision \$HeadURL \$LastChangedDate. If several tags should be placed, one can set up several keywords for a particular file:

```
svn propset svn:keywords "Id Date Revision HeadURL LastChangedDate" file_name.f90
```

Check out full documentation in the SVN manual about propset and svn:keyword.

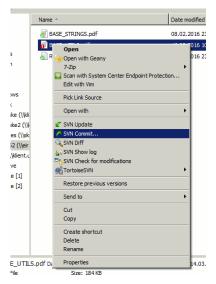


## **Important**

Subversion keywords are case sensitive, so \$ID or \$id won't work.

## 4.5 GUI Tools

Using the GUI tools like TortoiseSVN is similar to using the terminal commands. With GUI you should just select the appropriate item from the menu list.



Initial setup for the repository in TortoiseSVN is simple.

Checking changes, diff-ing, setting properties and keywords etc. is also very easy and visual with the built-in tool. Another useful feature is the revision graphs showing sequence of versions and pattern of branching. TortoiseSVN is incorporated into the Windows explorer and uses small overlay icons to show the status of the files and directories.

Similar GUI tools, although not as mature as TortoiseSVN, exist for Linux. For example, there is thunar-vcs-plugin (Git and Subversion integration into the Thunar file manager).



Subversion also integrates with numerous other tools, e.g. there is an SVN plugin for the Geany editor, plugins for the Microsoft Visual Studio IDE etc. Do not forget that version control systems are not only for just program code but any text-based files. So writing papers in LaTeX benefits from a built-in Subversion support in the TexStudio. There is even integration for Microsoft Office although non-free.

# 5 Object-oriented programming and modelling

## 5.1 General principles

Modern Fortran (2003 and 2008 standards) allows coding in a true object-oriented style, although does not require it. Object oriented style allows to define user's abstractions that mimic real world objects, isolate extra complexity of the objects and create extensions of objects.

Object oriented programming is based on the following principles:

**Abstraction:** defining and abstracting common features of objects and functions.

**Modularity and hiding irrelevant information:** An object is written and treated separately from other objects. Details about internal functioning of the object are effectively hidden, what is important is the *interface* of the object, i.e. how it interacts with the external world. This reduces complexity.

**Encapsulation:** combining components of the object to create a new object.

**Inheritance:** components of objects (both data and functions) can be inherited across objects, e.g. properties the "genome" object inherited by a more general object "the individual."

**Polymorphism:** the provision of a single interface to objects of different types.

At the most basic level the programmer defines both the **data structure** (user's type) as well as the types of **operations** (subroutines and functions) that are linked with and are be applied to the data structure.

#### **Important**



Object-oriented features of Fortran are described in recent Fortran books, e.g.: **Brainerd**, **W.S.** (2009). *Guide to Fortran 2003 Programming*, Springer (Chapter 12). **Chapman**, **S.J.** (2007) *Fortran 95/2003 for Scientists and Engineers*, 3rd ed., McGraw-Hill (Chapter 16). **Chivers**, **I. & Sleightholme**, **J.** (2012) *Introduction to Programming with Fortran: With Coverage of Fortran 90*, 95, 2003, 2008 and 77, Springer (Chapter 26). Short introduction can also be found on the internet, e.g. **Leai**, **M.** *Object-oriented programming in Fortran 2003* (PGI: www.pgroup.com). Part 1: Code Reusability; Part 2: Data Polymorphism.

## 5.2 Implementation of objects

It is the most convenient and natural to define a single object or closely related objects within the same Fortran module. Note also that components of an object or derived type are referred using the percent symbol %, e.g. fish%sex refers to a component sex of the object fish. Both derived type data components and functions are referred in this way. Derived type data objects can be combined into arrays as "normal" data. For example, the sex component of the *i*-th element of the array of derived type fish is referred as fish(i)%sex. Note that derived types can also include arrays, so predator%prey(j) can be *j*-th element of the prey array component of the object predator. If we use an array of derived type that includes a three-dimensional array component, it could be something like fish(i)%position(x,y,z).

Data structure (user-defined type) is defined in Fortran using the keywords: type ... end type. An object can also include subroutines and/or functions. For example, the following object INDIVIDUAL\_GENOME includes a data structure consisting of a single character string str and two subroutines that define its behaviour. The first subroutine has the internal name init\_genome\_random but is referenced outside of the object as init\_genome (i.e. init\_genome is a part of the object's interface').

```
private :: init_genome_random, mutate_genome ! Internal names are "private," so
! the outside procedures can refer
! the object subroutines by their
! outer "interface" names set on
contains ! the left of "=>"

subroutine init_genome_random(this) ! The subroutine is almost as usual
class(INDIVIDUAL_GENOME) :: this ! Note the use of the CLASS keyword
......
end subroutine init_genome_random
....
end module THE_GENOME
```

Note that the subroutine part of the object init\_genome\_random must have an item of the type definition (this) as its first argument. However, we must define it as class() rather than type(). With class, the subroutine will work not only with this specific type, but also with any of its extension (i.e. it is a polymorphic type).

We may then define an additional, more general, object extending the <code>INDIVIDUAL\_GENOME</code>. In this case, we use the word <code>extends</code> in the new type definition (see code below). This says that the components of the <code>INDIVIDUAL\_GENOME</code> are also included into the new object <code>INDIVIDUAL\_NEURO\_ARCH</code> (i.e. <code>INDIVIDUAL\_NEURO\_ARCH</code> inherits the <code>INDIVIDUAL\_GENOME</code> components).

```
module THE_NEUROBIO
.....
type, public, extends(INDIVIDUAL_GENOME) :: INDIVIDUAL_NEURO_ARCH
  integer :: bundles
  contains
    procedure, public :: init_neuro => init_neurobio_random
end type INDIVIDUAL_NEURO_ARCH

private :: init_neurobio_random

contains

subroutine init_neurobio_random(this)
    class(INDIVIDUAL_NEURO_ARCH) :: this
    .......
end subroutine init_neurobio_random
```

In this way, it is easy to create new objects inheriting properties of other objects, for example, create several layers ranging from the **genome** through the **neurobiological architecture** and up to the **individual fish** and further to a **population** of fish.

However, the above is just the *definition* of an object. To use the object, we must *instantiate* it, i.e. create its specific instance and set the values. This is analogous to having a specific data type, e.g. integer. We cannot use "just an integer," we need (1) to create a specific variable (variable is also an object though trivial!) of the type *integer* (e.g. integer :: Var\_A) and (2) to assign a specific value to it (Var\_A=1).

For example, the following creates two instance arrays of the type INDIVIDUAL\_FISH. Both arrays are one-dimensional and have POPSIZE elements. So we now have two fish populations, generation\_one and generation\_two. Each individual value of such an array, e.g. generation\_one(1) is an instance of the object of the type INDIVIDUAL\_FISH that can be quite a complex data structure including many different data types, even arrays and lower-order derived types (you can define derived types inside other derived types). So, instead of being arrays of simple values these object arrays are in fact arrays of complex data structures potentially consisting of many different data types and arrays:

```
type(INDIVIDUAL_FISH), dimension(POPSIZE) :: generation_one
type(INDIVIDUAL_FISH), dimension(POPSIZE) :: generation_two
```

We can now assign concrete values to each of the previously defined components of generation\_one array, e.g.

```
generation_one(i)%sex = "male" ! assign values to individual components
generation_one(i)%alive = .true. ! of the object instance
generation_one(i)%food(j) = "spaghetti"
```

We can also use the subroutines and type-bound functions that we have defined within the object definitions to do specific manipulations on the object and its components:

TODO - more text later

## 6 Introduction to the AHA Fortran modules

Module is just a piece of Fortran program that contains variable or constant declarations and functions and subroutines. Modules are defined in such a simple way:

To use any variable/constant/subroutine/function from the module, the program must include the use MODULE\_NAME statement:

```
use SOME_MODULE
....
```

The AHA modelling tools include several separate modules:

- BASE\_UTILS
- CSV\_IO
- BASE\_RANDOM
- BASE STRINGS
- LOGGER
- Error trapping modules
- IEEE Arithmetics modules

BASE\_UTILS contains a few utility functions. CSV\_IO is for output of numerical data into the CSV (comma separated values) format files. CSV is good because it is human-readable but can still be easily imported into spreadsheets and stats packages (R reads CSV). It also has little file size overhead which is good if huge amounts of data are generated by the model.

Invoking the modules requires the use keyword in Fortran. use should normally be the first statements before implicit none:

Building the program with these modules using the command line is normally a two-step process:

build the modules, e.g.

```
gfortran -g -c ../BASE_CSV_IO.f90 ../BASE_UTILS.f90
```

This step should only be done if the source code of the modules change, i.e. quite rarely.

build the program (e.g. TEST.f90) with these modules

```
gfortran -g -o TEST.exe TEST.f90 ../BASE_UTILS.f90 ../BASE_CSV_IO.f90
```

or for a generic F95 compiler:

```
f95 -g -c ../BASE_CSV_IO.f90 ../BASE_UTILS.f90
f95 -g -o TEST.exe TEST.f90 ../BASE_UTILS.f90 ../BASE_CSV_IO.f90
```

A static library of the modules could also be built, so the other more changeable code can be just linked with the library.



#### Note

The examples above assume that the module code is located in the upper-level directory, so ../, also the build script or Makefile should normally care about all this automatically.

# 7 Module: BASE\_UTILS

This module contains a few utility functions and subroutines. So far there are two useful things here: **STDOUT**, **STDERR**, **TOSTR**, **CLEANUP**, and **RANDOM\_SEED\_INIT**.

#### 7.1 Function: TOSTR

**TOSTR** converts everything to a string. Accepts any numeric or non-numeric type, including integer and real (kind 4 and 8), logical and strings. Also accepts arrays of these numeric types. Outputs just the string representation of the number. Aliases: **STR** (same as **TOSTR**), **NUMTOSTR** (accepts only numeric input parameter, not logical or string)

#### 7.1.1 Examples:

#### Integer:

```
STRING = TOSTR(12)
produces "12"
```

Single precision real (type 4)<sup>2</sup>

```
print *, ">>", TOSTR(3.1415926), "<<"
produces >>3.14159250<</pre>
```

Double precision real (type 8)

```
print *, ">>", TOSTR(3.1415926_8), "<<"
produces >>3.1415926000000001<<</pre>
```

TOSTR also converts logical type to the "TRUE" or "FALSE" strings and can also accept character string as input. In the latest case it just output the input.

### **Optional parameters**

TOSTR can also accept standard Fortran format string as the second optional **string** parameter, for example:

```
produces >>3.14<</pre>
print *, ">>", TOSTR(12,"(i4)"), "<<"
```

```
print *, ">>", TOSTR(12,"(i4)"), "<<"
produces >> 12<<</pre>
```

With integers, TOSTR can also generate leading zeros, which is useful for auto-generating file names or variable names. In such cases, the number of leading zeros is determined by the second optional **integer** parameter. This integer sets the template for the leading zeros, the maximum string. The exact value is unimportant, only the number of digits is used.

For example,

```
print *, ">>", TOSTR(10, 100), "<<"
produces >>010<</pre>
```

```
print *, ">>", TOSTR(10, 999), "<<"
also produces >>010<</pre>
```

```
print *, "File_" // TOSTR(10, 10000) // ".txt"
produces File_00010.txt
```

## **Examples of arrays**

It is possible to convert numeric arrays to their string representation:

print \*, ">>", TOSTR(3.1415926,"(f4.2)"), "<<"</pre>

```
real, dimension(6) :: RARR = [0.1,0.2,0.3,0.4,0.5,0.6]
....
print *, ">>", TOSTR(RARR), "<<"
produces > 0.100000001 0.200000003 0.300000012 0.400000006 0.5000000000 0.600000024<</pre>
```

Fortran format statement is also accepted for arrays:

```
real, dimension(6) :: RARR = [0.1,0.2,0.3,0.4,0.5,0.6]
....
print *, ">>", TOSTR(RARR,"(f4.2)"), "<<"
produces >> 0.10 0.20 0.30 0.40 0.50 0.60<</pre>
```

<sup>&</sup>lt;sup>2</sup> Note that float point calculations, especially single precision (real type 4) may introduce a rounding error

It is possible to use array slices and array constructors with implicit do:

```
print *, ">>", TOSTR(RARR(1:4)), "<<"
print *, ">>", TOSTR( (/(RARR(i), i=1,4)/) ), "<<"
both produce >> 0.100000001 0.200000003 0.300000012 0.400000006<<</pre>
```

or using the newer format with square brackets:

```
print *, ">>", TOSTR( [(RARR(i), i=1,4), 200.1, 400.5] ), "<<"
produces >> 0.100000001 0.200000003 0.300000012 0.400000006 200.100006 400.500000<</pre>
```

the same with format:

```
print *, ">>", TOSTR( [(RARR(i), i=1,4), 200.1, 400.5], "(f9.3)" ), "<<"
produces >> 0.100 0.200 0.300 0.400 200.100 400.500<</pre>
```

The subroutine TOSTR is useful because it allows to change such confusing old-style Fortran string constructions as this

```
!print new gene pool. First make file name
                                                !BSA 18/11/13
if (gen < 10) then
 write(gen1,2902) "gen-0000000",gen
else if (gen < 100) then
 write(gen1,2903) "gen-0000000",gen
else if (gen < 1000) then
 write(gen1,2904) "gen-000000",gen
else if (gen < 10000) then
 write(gen1,2905) "gen-00000",gen
else if (gen < 100000) then
 write(gen1,2906) "gen-0000", gen
else if (gen < 1000000) then
 write(gen1,2907) "gen-000",gen
else if (gen < 10000000) then
 write(gen1,2913) "gen-00",gen
else if (gen < 100000000) then
 write(gen1,2914) "gen-0",gen
else
 write(gen1,2915) "gen-",gen
end if
if (age < 10) then
 write(gen2,2920) "age-0000",age
else if (age < 100) then
 write(gen2,2921) "age-000",age
else if (age < 1000) then
 write(gen2,2922) "age-00",age
else if (age < 10000) then
 write(gen2,2923) "age-0",age
else
 write(gen2,2924) "age-",age
end if
write(gen3,2908)gen1,"-",gen2
if (expmt < 10) then
 write(string104,2901)"HED24-",MMDD,runtag,"-E0",expmt,"-o104-genepool-",gen3,".txt"
 write(string104,2910)"HED24-",MMDD,runtag,"-E",expmt,"-o104-genepool-",gen3,".txt"
end if
```

to a much shorter and clear like this:

```
!print new gene pool. First make file name !BSA 18/11/13
```

## 7.2 Subroutines: STDOUT and STDERR

These subroutines output arbitrary text to the terminal, either to the standard output and standard error. While it seems trivial (standard Fortran print \*, or write() can be used), it is still good to have a dedicated standard subroutine for all outputs as we can then easily modify the code to use Matlab/R API to work with and run models from within these environments, or use a GUI window (the least necessary feature now, but may be useful if the environment is used for teaching in future). In such cases we will then implement a specific dedicated output function and just globally swap STDOUT with something like R\_MESSAGE\_PRINT or X\_TXTGUI\_PRINT.

**STDOUT/STDERR** accept an arbitrary number of string parameters, which just represent messages placed to the output. Each parameter is printed on a new line. Trivial indeed:)



#### **Important**

It is useful to have two separate subroutines for stdout and stderr as they could be easily separated (e.g. redirected to different files). Redirection could be done under Windows/Linux terminal in such a simple way:

```
model_command.exe 1>output_file_stdout 2>output_file_stderr
Here STDOUT is redirected to output file stdout, STDERR, to output file stderr.
```

#### **Examples**

```
call STDOUT("-----", & ch01 // " = " // ch02 // TOSTR(inumber) // " ***", & ch10 // "; TEST NR= " // TOSTR(120.345), & "Pi equals to = " // TOSTR(realPi, "(f4.2)"), & "-----")
```

The above code just prints a message. Note that TOSTR function is used to append numerical values to the text output (unlike standard write where values are separated by commas).

#### 7.3 Function: CLEANUP

**CLEANUP** Removes all spaces, tabs, and any control characters from the input string. It is useful to make sure there are no trailing spaces in fixed Fortran strings and no spaces in file names.

#### Example:

```
print *, ">>", CLEANUP("This is along string blablabla"), "<<"
produces >>Thisisalongstringblablabla<<</pre>
```

## 7.4 Subroutine: RANDOM\_SEED\_INIT\_SIMPLE

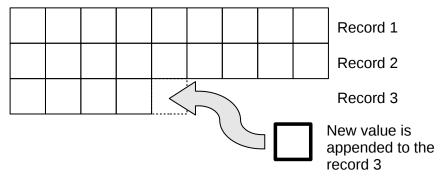
**RANDOM\_SEED\_INIT\_SIMPLE** is called without parameters and just initialises the random seed for the Fortran random number generator. But note that the module BASE\_RANDOM contains a much better subroutine RANDOM\_SEED\_INIT that is also suitable for parallel processing systems (RANDOM\_SEED\_INIT\_SIMPLE **cannot** be used in parallel calculations).

```
call RANDOM_SEED_INIT
```

# 8 Module: CSV\_IO

#### 8.1 Overview

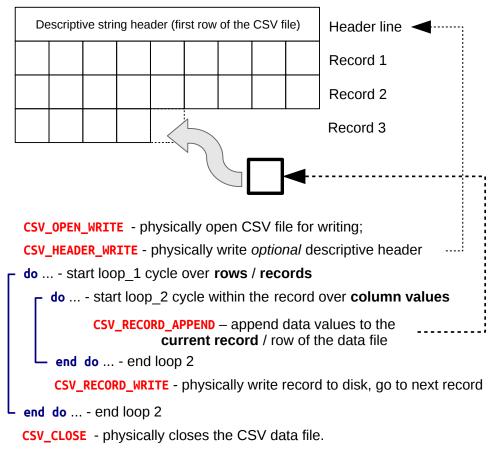
This module contains subroutines and functions for outputting numerical data to the CSV (Comma Separated Values) format (RFC4180, CSV format). There are now only routines for data output to CSV, not (yet?) for input as we don't input much data. CSV **record** is a whole line (**row**) of numbers/strings (as in Excel), a single file can have quite many records (rows).



For example, records (rows) can represent consecutive **generations** during the evolution or **individuals** for within-generation data.

In a typical workflow, within-column variables (i.e those that belong to the same row of data file) are appended to the same record. When the record is full (i.e. the number of values appended is equal to the number of columns in the CSV file), the record is written physically to the disk file and we can go to writing the next record (row) of the data.

Such a workflow can be like this:



Thus, subs ending with **\_WRITE** and **\_CLOSE** do physical write.

This module is most suited at this moment for CSV file *output* rather than input.

This module widely uses **optional arguments**. They may or may not be present in the function/subroutine call. If not all parameters are passed, so called *named parameters* are used. That is, the name of the parameter(s) within the function is explicitly stated when the function/subroutine is called.

For example, GET\_FREE\_FUNIT has its both parameters optional (max\_funit and file\_status), it can be called in the standard way as below:

```
intNextunit = GET_FREE_FUNIT(200, logicalFlag)
```

It can lack any parameter:

```
intNextunit = GET_FREE_FUNIT()
```

If the first optional parameter is absent, GET\_FREE\_FUNIT is called as here:

```
intNextunit = GET_FREE_FUNIT(file_status=logicalFlag)
```

If both parameters present but swapped in order, it should be

```
intNextunit = GET_FREE_FUNIT(file_status=logicalFlag, max_funit=200)
```

of course, it can also be used this way:

```
intNextunit = GET_FREE_FUNIT(max_funit=200, file_status=logicalFlag)
```



#### **Important**

The standard way of using subroutine parameters (without explicitly setting their names) when calling subroutine works only when their are not missing and their order remains the same as in the subroutine declaration. When a function / subroutine has many parameters and optional are interspersed with mandatory, *it is probably just safer to use named parameters anyway*.

Files can be referred either by unit or by name, but unit has precedence (if both a provided, unit is used). There is also a derived type **csv\_file** that can be used as a single file handle. If csv\_file object is defined, the file name, unit and the latest operation success status can be accessed as %name, %unit, %status (e.g. some\_file%name, some\_file%unit).

The physical file operation error flag, csv\_file\_status is of logical type. It is always an optional parameter.

Here is an example of the data saving workflow:

```
use CSV_IO ! invoke this module first
. . . . . . . .
! 1. Generate file name for CSV output
csv_file_append_data_name="data_genomeNR_" // TOSTR(i) // "_" // TOSTR(j) // &
                           "_" // TOSTR(k) // ".csv"
! 2. open CSV file for writing
call CSV_OPEN_WRITE (csv_file_append_data_name, csv_file_append_data_unit, &
                     csv_written_ok)
if (.not. csv_written_ok) goto 1000 ! handle possible CSV error
! 3. Write optional descriptive header for the file
call CSV_HEADER_WRITE(csv_file_name = csv_file_append_data_name, &
                      header = header_is_from_this_string, &
                      csv_file_status = csv_written_ok)
. . . . . . . .
. . . . . . . .
! 4. Generate a whole record of variable (column) names
record_csv="" ! but first, prepare empty record string
call CSV_RECORD_APPEND(record_csv,["VAR_001", ("VAR_" // TOSTR(i,100),i=2,Cdip)])
! 5. physically write this variable header record to the file
```

```
call CSV_RECORD_WRITE (record=record_csv, &
                       csv_file_name=csv_file_append_data_name, &
                       csv_file_status=csv_written_ok)
if (.not. csv_written_ok) goto 1000 ! handle possible CSV error
. . . . . . . .
! 6. Now we can write records containing actual data values, we do this
! in two do-cycles
CYCLE_OVER_RECORDS: do l=1, Cdip
  ! 7. Prepare an empty string for the current CSV record
  record_csv=""
  CYCLE_WITHIN_RECORD: do m=1, CNRcomp
    . . . .
    ! do some calculations...
    ! 8. append the next value (single number: genomeNR) to the current record
    call CSV_RECORD_APPEND ( record_csv, genomeNR(1,m) )
  end do CYCLE_WITHIN_RECORD
  ! 9. physically write the current record
  call CSV_RECORD_WRITE ( record=record_csv, &
                          csv_file_name=csv_file_append_data_name, &
                          csv_file_status=csv_written_ok )
 if (.not. csv_written_ok) goto 1000 ! handle possible CSV error
  . . . . . . .
end do CYCLE_OVER_RECORDS
! 10. close the CSV file when done
call CSV_CLOSE( csv_file_name=csv_file_append_data_name, &
                csv_file_status=csv_written_ok )
if (.not. csv_written_ok) goto 1000 ! handle possible CSV error
```

Although, there is a wrapper for saving the whole chunk of the data at once. A whole array or matrix (2-dimensional table) can be exported to CSV in a single command:

```
! save the whole matrix/array d_matrix to some_file.csv
call CSV_MATRIX_WRITE(d_matrix, "some_file.csv", fstat_csv)
if (.not. fstat_csv) goto 1000
```

## 8.2 Subroutine: CSV\_OPEN\_WRITE

Open CSV file for writing. May have two forms:

(1) either get three parameters:

```
character (len=*) :: csv_file_name ! file name
integer :: csv_file_unit ! file unit
logical :: csv_file_status ! optional status flag, TRUE if operation
! successful
```

(2) get the (single) file handle object of the derived type csv\_file

```
type(csv_file), intent(inout) :: csv_file_handle ! file handle object
```

```
type(csv_file) :: file_occ    ! declare file handle object
......
call CSV_OPEN_WRITE(file_occ)   ! use file handle object
......
call CSV_OPEN_WRITE(file_name_data1, file_unit_data1, fstat_csv)  ! old style
if (.not. fstat_csv) goto 1000
```

## 8.3 Subroutine: CSV\_CLOSE

Closes a CSV file for reading or writing. May have two forms:

(1) either get three optional parameters:

```
character (len=*) :: csv_file_name ! file name
integer :: csv_file_unit ! file unit
logical :: csv_file_status ! optional status flag, TRUE if operation
! successful
```



## **Important**

At least **file name** or **unit** should be present in the subroutine call.

(2) get one file handle object of the derived type csv\_file

```
type(csv_file), intent(inout) :: csv_file_handle ! file handle object
```

### Example

## 8.4 Subroutine: CSV\_HEADER\_WRITE

Writes an optional descriptive header to a CSV file. The header should normally be the first line of the file.

May have two forms:

(1) either get four parameters, only the header is mandatory, but the file must be identified by name or unit:

```
character (len=*) :: csv_file_name ! file name
integer :: csv_file_unit ! file unit
character (len=*) :: header ! header string
logical :: csv_file_status ! status flag, TRUE if operation successful
```



#### **Important**

At least **file name** or **unit** should be present in the subroutine call.

(2) get two parameters including the header string and the file handle object of the type csv\_file

```
call CSV_HEADER_WRITE(csv_file_name=FILE_NAME_CSV1, &
    header="Example header. Total " // TOSTR(CSV_RECORD_SIZE(record_csv)) // &
    " columns of data.", csv_file_status=fstat_csv)
if (.not. fstat_csv) goto 1000
```

Here CSV file header is generated from several components, including the  $CSV\_RECORD\_SIZE$  function to count the record size.

## 8.5 Function: GET\_FILE\_UNIT

Returns file unit associated with an existing open file name, if no file unit is associated with this name (file is not opened), return unit=-1 and error status

Input parameters:

```
character (len=*) :: csv_file_name ! mandatory file name
logical :: csv_file_status ! optional status flag, TRUE if operation
! successful
```

Output parameter (function value):

## Example

```
file_unit = GET_FILE_UNIT(file_name)
```

## 8.6 Function: GET\_FREE\_FUNIT

Returns the next free/available Fortran file unit number. Can optionally search until a specific maximum unit number.

Input parameters, optional:

Output parameter (function value):



## **Important**

When optional input parameters are absent, the function uses a hardwired maximum unit number, possibly depending on the computer platform and compiler used.

```
restart_file_unit_27 = GET_FREE_FUNIT()
```

## 8.7 Function: CHECK\_UNIT\_VALID

Checks if file unit is valid, that is within the allowed range and doesn't include standard input/output/stderr units. The unit should not necessarily be linked to any file or be an open file.

Input parameter:

Output parameter (function value):

#### Example

In this example, we check if the user provided unit is valid, if not, get the first available one.

## 8.8 Function: CHECK\_FILE\_OPEN

Checks if a file is currently open, can optionally determine the Fortran unit associated with an open file (returns -1 if it is not open). Input parameters can be either raw form (file name or unit) or csv\_file object. Optional csv\_file\_status can determine if the check proceeded without error (=TRUE) there was an error when trying to access the file (=FALSE). Input parameters must be either file name or unit.

Standard (verbose) form:

```
! Calling parameters
character (len=*), optional, intent(in) :: csv_file_name ! file name to check
integer, optional, intent(in) :: csv_file_unit ! or unit to check
logical, optional, intent(out) :: csv_file_status ! error status
integer, optional, intent(out) :: get_csv_file_unit ! obtain file unit of
! an open file
```

File object form:

```
type(csv_file) :: csv_file_handle
```

Output of the function is logical type, returns TRUE if the file is currently opened, FALSE otherwise.

#### **Examples:**

```
type (csv_file) :: output_handle
...
if (CHECK_FILE_OPEN(output_handle)) then
...
```

## 8.9 Subroutine: CSV\_RECORD\_APPEND

Appends one of the possible data objects to the current CSV record. Data objects could be either a single value (integer, real with single or double precision, character string) or a one-dimensional array of the above types or still an arbitrary length list of the same data types from the above list.

#### 8.9.1 Overview

The first parameter of the subroutine is always character string record:

```
character (len=*) :: record ! character string record to append data
```

The other parameters may be of any of thee following types: integer (kind=4), real(kind=4), real(kind=8), character string.



### **Important**

The record keeping variable can be either fixed length string or an allocatable string. But it should fit the whole record. This might be a little bit tricky if record is allocatable as record\_string="" allocates it to an empty string. A good tip is to use the repeat function in Fortran to allocate the record string to the necessary value, e.g. record=repeat(" ", MAX\_RECORD) will produce a string consisting of MAX\_RECORD blank characters. record should not necessarily be an empty string initially, it could be just a whole blank string.

#### 8.9.2 Examples

Append a single string to the current record:

```
call CSV_RECORD_APPEND(record_csv, "ROW_NAMES")
```

Append a single value (any of the supported types) to the current record:

```
call CSV_RECORD_APPEND(record_csv, value) ! some variable of supported type
call CSV_RECORD_APPEND(record_csv, 123.5_8) ! double precision literal value
```

Append a list of values (any one of the supported types) to the current record:

```
call CSV_RECORD_APPEND(record_csv, fish, age, stat4, fecund)
```

Append an array slice (any of the supported types) to the current record:

```
call CSV_RECORD_APPEND(record_csv, RARR(1:4))
```

Append an array using old-style array constructor with implied do (any of the supported types) to the current record:

```
call CSV_RECORD_APPEND(record_csv,(/(RARR(i), i=1,6)/))
```

Append an array using new-style array constructor (square brackets) with implied do plus two other values (all values can have any of the supported types but should have the same type) to the current record:

```
call CSV_RECORD_APPEND(record_csv, [(RARR(i), i=1,4), measur1, age(fish)])
```

Append integers from 1 to 10 to the current record (using implied do):

```
call CSV_RECORD_APPEND(record_csv, [(i,i=1,10)])
```

Append a string, an array of strings with implied do and finally another string to the record. This example shows how variable (column) names could be generated:

call CSV\_RECORD\_APPEND(record\_csv,["ROW\_NAME",("VAR\_" // TOSTR(i,1000),i=1,1000),"STATUS"])



#### **Important**

On some compilers (e.g. Oracle Solaris Studio f95 v.12 but not GNU gfortran version >5), all strings within the array constructor must explicitly have the same length, otherwise the compiler issues an error. In gfortran (v>5, the first occurrence of the string (e.g. the first iteration of the implied do loop) defines the default length and all extra characters are just silently dropped. The behaviour of other compilers and their versions may differ.

# 8.10 Function: CSV\_GUESS\_RECORD\_LENGTH

Guesses the maximum size for the string variable keeping the record being appended for CSV\_RECORD\_APPEND.

It gets two parameters: integer record size (the number of separate numerical values in the record) and the maximum target value (integer, real, or double precision real (kind=8)) and returns an integer value for a guess for the record size. The target value is used to estimate the number of characters and should have the same type as the values being appended with CSV\_RECORD\_APPEND.

```
! suppose we have a real matrix and like to save it to a CSV file
real, dimension(1000,20) :: MATRX_A
...
! we declare the CSV record as allocatable string
character(len=:), allocatable :: record_for_csv
...
! As explained in the Important note to CSV_RECORD_APPEND above, we have to
! allocate the string record such that it fits the complete record;
! This can be achieved as follows. Here 20 is the record size (number of cols,
! can be determined as ubound(MATRX_A,2)), and the target value is the
! maximum numeric value of the matrix MATRX_A:
record_for_csv = repeat(" ", CSV_GUESS_RECORD_LENGTH(20, maxval(MATRX_A)))
```



#### **Important**

Use this function with caution, especially if long strings are also added to the CSV file. In such a case, make additional allowance for the added string(s).

# 8.11 Function: CSV\_RECORD\_SIZE

Counts the number of values in a CSV record.

Input parameters:

```
character (len=*) :: record ! mandatory CSV record
```

Function value: an integer

```
integer :: csv_record_size
```

### Example

```
print *, "This record is: ", CSV_RECORD_SIZE(record_csv), " columns."
```

# 8.12 Function: CSV\_FILE\_LINES\_COUNT

Counts the number of lines in an existing CSV file. If file cannot be opened or file error occurred, then issues the value -1 Input parameters:

```
character (len=*) :: csv_file_name ! The name of the existing file
logical :: csv_file_status ! optional file operation status, TRUE if
! file operations were successful.
```

Function value: an integer

```
integer :: csv_file_lines_count    ! number of lines in file, -1 if file error
```

Can actually calculate the number of lines in any text file. Does not distinguish header or variable names lines in the CSV file and does not recognize CSV format.

#### Example

```
print *, "File ", CSV_FILE_LINES_COUNT("test_file.csv", succ_flag), "lines."
```

# 8.13 Subroutine: CSV\_RECORD\_WRITE

Physically writes a complete record of data to a CSV file. A record is a single row of data in the file.

This subroutine has two forms:

(1) it can either accept three parameters:



#### **Important**

The file to write the current record can be referred either by name or unit. So one of them must be present in the subroutine call.

(2) get the CSV record and the (single) file handle object of the derived type csv\_file

#### Example

Note, that file handle object is used in the above example.

# 8.14 Subroutine: CSV\_MATRIX\_WRITE

Writes a matrix of real (kind 4 or 8), integer or string values to a CSV data file. This is a shortcut allowing to write data in a single code instruction. This subroutine works either with a two-dimensional matrix or one-dimensional array (vector). The behaviour is a little different in these cases.

#### 8.14.1 Two-dimensional matrix

It gets the following parameters: (1) two-dimensional data matrix (of any supported type), (2) mandatory name of the output file; (3) optional vector of column names. If the column name vector is shorter than the "column" dimension of the data matrix, the remaining columns get "COL\_XXX" names, where XXX is the consecutive column number (so they are unique). and (4) optional logical file operation success status.

```
[any supported], dimension(:,:) :: matrix ! data object, array or 2-d matrix
character (len=*) :: csv_file_name ! file name for output
character, dimension(:) :: colnames ! optional array of column names
logical :: csv_file_status ! operation status, TRUE if success
```

### **Example**

**Higher-rank arrays** (with more than two dimensions)<sup>3</sup> can be saved into CSV files using array slices, for example:

#### 8.14.2 One-dimensional arrays

With one-dimensional array (vector), the subroutine gets (1) the array, (2) output file name, (3) logical parameter pointing if the array is saved "vertically" (as a single column, if TRUE) or "horizontally" (as a single row, if FALSE). If the vertical parameter is absent, the default TRUE (i.e. "vertical" data output) is used. There is also an alias to this subroutine, **CSV\_ARRAY WRITE**.

<sup>&</sup>lt;sup>3</sup> CSV\_IO code could be modified to save higher-rank arrays if this function is needed

#### **Example**

```
! Here the data will be written into a single row of values call CSV_MATRIX_WRITE (ARRAY, "data_file.csv", .FALSE., fstat_csv) if (.not. fstat_csv) goto 1000
```

#### Tip

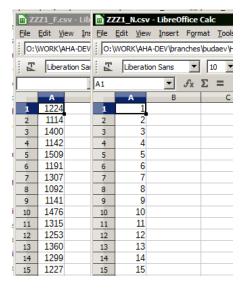
In the simplest cases, with only the data object and the file name, CSV\_MATRIX\_WRITE can be used with a two-dimensional matrix or one-dimensional array in the same way (it's convenient during debugging):

#### 8.14.3 Combining multiple arrays with RESHAPE

RESHAPE is a powerful Fortran function that allows combining several arrays in various ways. This could be very useful for saving multiple vectors (or arrays) of the same type into a single CSV file using a single line of code.

Suppose we have two integer object vectors generation\_one%individual%fitness and generation\_one%individual%person\_number each having POPSIZE elements (these are just two one-dimensional vector components of a single object). Each of these vectors can be saved using the standard CSV\_MATRIX\_WRITE call:

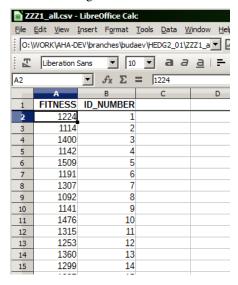
```
call CSV_MATRIX_WRITE (generation_one%individual%fitness, "ZZZ1_F.csv")
call CSV_MATRIX_WRITE (generation_one%individual%person_number, "ZZZ1_N.csv")
```



The code below reshapes these two vectors into a single two-column matrix (by columns, array constructors are in square brackets []), so in the final CSV file they represent two separate variables. Note that there is also an array constructor for two descriptive column names of the same string length.

```
["FITNESS ","ID_NUMBER"] &
```

So the resulting data CSV file is like this:



If the arrays to be combined have different types, it is possible to use whole-array type conversions to get some common type for all of the arrays. For example, if we combine an integer array A and a real array B (both having POPSIZE elements as above), it is wise to convert integer to real to avoid losing data precision:

We do not combine multiple loops manually, and automatic reshaping of the arrays is (usually) very fast.

# 8.15 Derived type: csv\_file

This type is used as a unitary file handle object. It has the following structure:

If csv\_file object is defined, the file name, unit and the latest operation success flag can be accessed as %name, %unit, %status (e.g. some\_file%name, some\_file%unit).

#### 8.15.1 Basic Example

#### 8.15.2 Arrays of structures

This derived type can be also used as an array. An example below shows how can this be done.

```
type(csv_file), dimension(:), allocatable :: file_ABM ! Define allocatable array
......
! of file handle objects
allocate(file_ABM(modulators)) ! Allocate this array
......
! now, use the array to handle many files of the same type
do j=1, modulators
  file_ABM(j)%name = "file_no_" // TOSTR(j,10) // ".csv" ! Set file handle (j)
  call CSV_OPEN_WRITE(file_ABM(j)) ! and use it
end do
```

#### **Important**



The file name is set as a standard **non-allocatable** fixed string because allocatable strings may not be supported on all compiler types and versions. Notably, older GNU gfortran (prior to v.5) does not allow allocatable strings in derived types. Currently, MAX\_FILENAME=255 (can be changed in the code). There is one consequence of using fixed strings: you may have to use the Fortran trim() function to cut off trailing blanks if strings are concatenated. E.g. do file\_name=trim(String1) //trim(String2) instead of file\_name=String1 //String2 or use file\_name=CLEANUP(String1 //String2) to remove all blank and control characters.

# 9 Module: BASE\_RANDOM

This module contains subroutines for generating random numbers (pseudo-random number generator, PRNG). However, the code of this module depends on the platform and compiler used. The build system (make) generates the appropriate header file automatically.

#### 9.1 Subroutine: RANDOM SEED INIT

Initialise the random seed for random number generation. This module uses an improved random seed generation algorithm that uses the system entropy pool on Unix systems and XOR of the current time and PID on Windows. Therefore, it is **safe** for use on **parallel processing systems**. Normally has no parameters.

```
call RANDOM_SEED_INIT()
```

RANDOM\_SEED\_INIT can optionally return the current (calculated) seed as two parameters: integer dimension of the seed array n\_here and the array itself seed\_here. This, however, is useful only for debugging.

The seed array size can be different: on GNU gfortran x86 it is 12, on Intel and Oracle Fortran (both x86) it is 2.

### 9.2 Function: RAND I

Generates a random integer (uniform distribution) within the range A to B (the two parameters of the function).

```
ipos = RAND_I(1, len(ga_target))
```

# 9.3 Functions: RAND\_R4 (RAND) and RAND\_R8

Generates a random real (kind 4 or 8) number with the *uniform* distribution. If the function has no parameters, it calculates a uniform random number ranging from **0** to **1**. May have two real or integer parameters defining the desired range (*minimum*, *maximum*) of the random numbers. RAND is an alias for RAND\_R4.

```
if ( RAND_R4() < ga_mutationrate ) then
   call mutate(fish(i))
end if
....
rate = RAND_R4(10,100) ! this generates a random number within 10..100</pre>
```

# (!)

#### **Important**

These functions are just wrappers to the standard Fortran subroutine random\_number. Note that such intrinsic Fortran functions as RAN are provided for backwards compatibility with the old *Fortran 77* standard. They are usually implemented as a simple modulo generator (as in £77). The new standard random\_number implements a superior algorithm and should be used for all new codes.

#### 9.4 Function: RNORM

In absence of any parameters, generates a normally distributed real (kind 4) random number with *zero mean* and *standard deviation* = 1.0. May also have two real parameters defining the desired *mean* and *variance*.

Based on algorithm 712, *Transactions on Mathematical Software*, 18, 4, 434-435 (1992); (Kinderman & Monahan, augmented with quadratic bounding curves).

```
ga_mutation = RNORM() ! generate Gaussian variate with mean 0 and variance 1
ga_i_length = RNORM(100.,10.) ! generate Gaussian variate with mean 100 and variance 10
```

# 9.5 Function: RAND\_STRING

Generates a string composed of random characters. It has a single mandatory integer parameter, the string length. There are also two optional integer parameters defining the range of the ASCII character codes for this string.

Some useful ranges: numbers 48:122, Latin alphanumeric characters 65:122, uppercase Latin letters 65:90, lowercase Latin letters: 97:122.

```
LABEL = RAND_STRING(24,97,122) ! Set a random label of 24 lowercase letters
```

# 9.6 Arrays of random numbers: RAND\_ARRAY and RNORM\_ARRAY

The subroutines RAND\_ARRAY and RNORM\_ARRAY generate arrays (up to 6-dimensions) of *uniform* and *normal (Gaussian)* random numbers, respectively. RAND\_ARRAY can generate real (kind=4) and integer arrays. In absence of additional parameters, RAND\_ARRAY produces values ranging within 0.0 and 1.0, RNORM\_ARRAY, normal (Gaussian) values with zero mean and unity standard deviation.

**Additional parameters for arbitrary random numbers.** As with the above single-value functions, additional parameters enable the generation of random numbers with arbitrary parameters. For example, two additional parameters of RAND\_ARRAY define the range (*minimum*, *maximum*) of uniformly distributed numbers whereas two additional parameters of RNORM\_ARRAY determines the *mean* and *variance* of the Gaussian random numbers generated.

The subroutine RAND\_ARRAY can be also used with an integer array as a parameter. In this case, the subroutine requires two additional integers that set the range of the integers generated.

There are aliases RAND\_MATRIX and RNORM\_MATRIX for two- to six-dimensional matrices.

Here are a few examples:

# 9.7 Build details

When **not using** the automatic build system based on GNU make, the module subroutine RANDOM\_SEED\_INIT should be tweaked according to the compiler and platform as follows:

#### **GNU fortran:**

#### **Intel Fortran**

#### **Oracle Fortran**

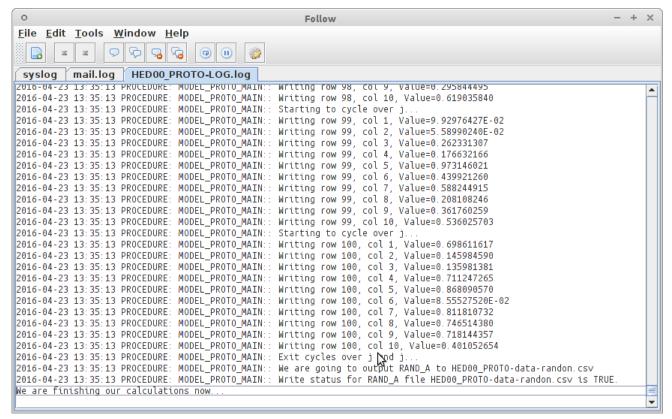
The build system based on GNU make does this automatically.

# 10 Module: LOGGER

### 10.1 Overview

This module controls logging arbitrary messages during the execution of the program. The format and destination of the messages is configurable during the run time. Thus, a trace of the execution can be read by the user during and after the execution. The module includes subroutines to connect a file to the logger, configure the logging process, for example enable or disable the terminal (stdout) messages, issue actual log messages. There are four log levels (**volume**, **chapter**, **section** and **subsection**) that can differ a little in the visual representation, it can be useful for marking specific parts of the log. Logging is especially useful for simulation models that run for quite a long time like AHA. The user can then check the log from time to time to make sure everything is in order and get an idea about where it is running now.

Here is an example of a log file with timestamps (date and time printed on the left of the log strings) being displayed using the Follow program.



# 10.2 Subroutine: LOG\_STARTUP

The logger must be started up with the subroutine LOG\_STARTUP that has the log file name as a parameter, for example call LOG\_STARTUP ("logfile-01.log"). The second optional argument defines if the existing log file with the same name should be appended (.TRUE., default) or overwritten (.FALSE.). The code below shows how to start logging and build the log file from parts:

# 10.3 Subroutine: LOG\_CONFIGURE

There are also several configuration options for the LOGGER which are called using the LOG\_CONFIGURE subroutine.

LOG\_CONFIGURE accepts two parameters:

- · character string parameter name
- parameter value (character string, integer or logical type)

These are the possible configuration options and their explanations:

Option	Value	Explanation
timestamp	logical TRUE/FALSE	if timestamp is issued in the log
writeonstdout	logical TRUE/FALSE	if the log should also go to terminal (stdout)
writeonlogfile	logical TRUE/FALSE	if the log should also go to the disk file
stoponerror	logical TRUE/FALSE	defines if execution should stop on error
logfileunit	integer value	Set specific unit for log (use with caution!)
level_string_volume	string delimiter	Set the string for <b>volume</b>
level_string_chapter	string delimiter	Set the string for <b>chapter</b>
level_string_section	string delimiter	Set the string for <b>section</b>
level_string_subsection	string delimiter	Set the string for <b>subsection</b>

The following code shows an example of LOGGER configuration. Here it turns **on** printing timestamps in the log and chooses whether log messages should also go to the screen terminal (stdout).

```
call LOG_CONFIGURE("timestamp", .TRUE.) ! do timestamps in the log

if (IS_DEBUG) then
   call LOG_CONFIGURE("writeonstdout" , .TRUE.) ! output also to screen if DEBUG
else
   call LOG_CONFIGURE("writeonstdout" , .FALSE.) ! NO screen log output normally
end if
```

# 10.4 Function: LOG\_ISINITIALIZED

The logical function LOG\_ISINITIALIZED returns TRUE if the logger is already initialised.

```
if (LOG_ISINITIALIZED) then
```

# 10.5 Subroutine: LOG\_CGET

The subroutine LOG\_CGET is used to query a LOGGER configuration option value. It has two parameters, character string option and logical, integer or character string value. Its use is similar to LOG\_CONFIGURE.

```
call LOG_CGET("writeonstdout", is_stdout) ! check if log is going to screen
```

# 10.6 Subroutine: LOG\_DELIMITER

LOG\_DELIMITER issues a string delimiter to the log, it has an optional integer argument setting the kind of the delimiter, default is "volume" (1). This is useful to mark the log with visually different parts. The maximum string length of the delimiter is **80** characters (set as a public integer parameter LOG\_LEVEL\_DELIMITER\_LENGTH).

The four levels of logging **volume**, **chapter**, **section** and **subsection** are defined in the module LOGGER as constants, so these constant can be used instead of the integer number. There are also the default delimiter strings.

Below is a code example of issuing log delimiters:

Using a user-defined delimiter string is illustrated below.

```
! Set delimiter as a 60-characters long line of "=====..." for volume delimiter

call LOG_CONFIGURE("level_string_volume", repeat("=",60))

......

call LOG_DELIMITER(LOG_LEVEL_VOLUME) ! issues this long delimiter line
```

### 10.7 Subroutine: LOG\_SHUTDOWN

LOG\_SHUTDOWN: The last thing to do is to shut down logging with the LOG\_SHUTDOWN subroutine:

```
call LOG_SHUTDOWN () ! close logger
```

# 11 Module: BASE\_STRINGS

This module containing some useful string manipulation functions is borrowed from <a href="http://www.gbenthien.net/strings/index.html">http://www.gbenthien.net/strings/index.html</a>. The description below is just repeating the official doc file included with the module. Note that there are a couple of utils (READLINE, WRITEQ) in this module that work with files. These use the standard Fortran unit to refer for the file and unlike the other modules here are not adjusted (yet) to use the file handle object (csv\_file).

Fortran Character String Utilities. A collection of string manipulation routines is contained in the module 'strings' found in the file stringmod.f90. To obtain this module as well as some other string utilities, go to the website <a href="http://www.gbenthien.net/strings/index.html">http://www.gbenthien.net/strings/index.html</a>. To use the routines in the module 'strings' the user needs to add the statement use strings to the top of the program. These routines were developed primarily to aid in the reading and manipulation of input data from an ASCII text file. The routines are described below.

# 11.1 Subroutine: PARSE

```
SUBROUTINE PARSE(str, delims, args, nargs)
```

This routine was originally designed to separate the arguments in a command line where the arguments are separated by certain delimiters (commas, spaces, etc.). However, this routine can be used to separate other types of strings into their component parts.

The first input is a string str (e.g., a command line). The second argument is a string delims containing the allowed delimiters. For example, delims might be the string ", " consisting of a comma and a space. The third argument is a character array args that contains on output the substrings (arguments) separated by the delimiters. Initial spaces in the substrings (arguments) are deleted. The final argument is an integer nargs that gives the number of separated parts (arguments). To treat a delimiter in str as an ordinary character precede it by a backslash (\). If a backslash character is desired in str, precede it by another backslash (\). In addition, spaces that immediately precede or follow another delimiter are not considered delimiters. Multiple spaces or tabs are considered as a single space, i.e., "a b" is treated the same as "a b". Backslashes can be removed from an argument by calling the routine REMOVEBKSL, i.e.,

```
call REMOVEBKSL(<string>)
```

This routine converts double backslashes (\\) to single backslashes (\).

**Example:** If the delimiters are a comma and a space (delims = ","), then the subroutine PARSE applied to the string "cmd arg1 arg12 arg3" produces the output:

```
args(1) = cmd
args(2) = arg1
args(3) = arg 2
args(4) = arg3
nargs = 4
```

# 11.2 Subroutine: COMPACT

```
SUBROUTINE COMPACT(str)
```

This routine converts multiple spaces and tabs to single spaces and deletes control characters.

#### 11.3 Subroutine: REMOVESP

```
SUBROUTINE REMOVESP (str)
```

This routine removes spaces, tabs, and control characters in string str.

# 11.4 Subroutine: VALUE

```
SUBROUTINE VALUE(str, number, ios)
```

This subroutine converts a number string to a number. The argument str is a string representing a number. The argument number is the resulting real number or integer (single or double precision). The argument ios is an error flag. If ios is nonzero, then there was an error in the conversion.

#### 11.5 Subroutine: SHIFTSTR

```
SUBROUTINE SHIFTSTR(str, n)
```

This routine shifts characters in the string str by n positions (positive values denote a right shift and negative values denote a left shift). Characters that are shifted off the end are lost. Positions opened up by the shift are replaced by spaces.

### 11.6 Subroutine: INSERTSTR

```
SUBROUTINE INSERTSTR(str, strins, loc)
```

This routine inserts the string strins into the string str at position loc. Characters in str starting at position loc are shifted right to make room for the inserted string.

#### 11.7 Subroutine: DELSUBSTR

```
SUBROUTINE DELSUBSTR(str, substr)
```

This subroutine deletes the first occurrence of substring substr from string str and shifts characters left to fill hole.

#### 11.8 Subroutine: DELALL

```
SUBROUTINE DELALL(str, substr)
```

This routine deletes all occurrences of substring substr from string str and shifts characters left to fill holes.

#### 11.9 Function: UPPERCASE

```
FUNCTION UPPERCASE (str)
```

This function returns a string that is like the string str with all characters that are not between a pair of quotes (" " or ' ') converted to uppercase.

#### 11.10 Function: LOWERCASE

```
FUNCTION LOWERCASE (str)
```

This function returns a string that is like the string str with all characters that are not between a pair of quotes (" " or ' ') converted to lowercase.

#### 11.11 Subroutine: READLINE

```
SUBROUTINE READLINE (nunitr, line, ios)
```

This routine reads a line from unit nunitr, ignoring blank lines and deleting comments beginning with an exclamation point(!). The line is placed in the string line. The argument ios is an error flag. If ios is not equal to zero, then there has been an error in the read operation. A negative value for ios denotes an end of file.

#### 11.12 Subroutine: MATCH

```
SUBROUTINE MATCH(str, ipos, imatch)
```

This routine finds the delimiter in string str that matches the delimiter in position ipos of str. The argument imatch contains the position of the matching delimiter. Allowable delimiters are  $(), [], \{\}, <$ .

#### 11.13 Subroutine: WRITENUM

```
SUBROUTINE WRITENUM (number, string, fmt)
```

This routine writes a number to a string. The argument number is a real number or an integer (single or double precision). The number number is written to the character string string with format fmt (e.g., "e15.6" or "i5").

#### 11.14 Subroutine: TRIMZERO

```
SUBROUTINE TRIMZERO(str)
```

This subroutine deletes nonsignificant trailing zeroes in a number string str. A single zero following a decimal point is allowed. For example, "1.50000" is converted to "1.5" and "5." is converted to "5.0".

#### 11.15 Subroutine: WRITEQ

SUBROUTINE WRITEQ(unit, name, value, fmt)

This routine writes a string of the form "name=value" to the unit unit. Here name is the input string name and value is the input number value converted to a string with the format fmt. The number value can be a real number or an integer (single or double precision).

# 11.16 Function: IS LETTER

FUNCTION IS\_LETTER (ch)

This function returns the logical value . TRUE. if the input character ch is a letter (a-z or A-Z). It returns the value .FALSE. otherwise.

# 11.17 Subroutine: IS DIGIT

FUNCTION IS\_DIGIT(ch)

This function returns the logical value .TRUE. if the input character ch is a digit (0-9). It returns the value .FALSE. otherwise.

#### 11.18 Subroutine: SPLIT

SUBROUTINE SPLIT(str, delims, before, sep)

This routine uses the first occurrence of a character from the string delims in the string str to split the string into two parts. The portion of str before the found delimiter is output in before; the portion of str after the found delimiter is output in str (str is left justified). The output character sep (optional) contains the found delimiter. To treat a delimiter in str as an ordinary character precede it by a backslash (\\). If a backslash is desired in str, precede it by another backslash (\\\). Repeated applications of SPLIT can be used to parse a string into its component parts. Backslashes can be removed by calling the routine REMOVEBKSL, i.e., call REMOVEBKSL (string)

# 12 IEEE Arithmetics

#### 12.1 Overview

The model can now use the IEEE arithmetic modules. They allow exact control of the CPU math features and exceptions caused by invalid calculations, such as dividion by zero, overflow, underflow etc. A potential issue is that they have an optional status in the Fortran standard, so compilers do not have to implement them, although many do.



#### **Important**

IEEE arithmetic and exceptions are fully described in chapter 14 of this book: Adams, et al., 2009 *The Fortran 2003 Handbook*. Springer.

For example, Intel Fortran implements intrinsic IEEE arithmetics modules. GNU Fortran does not implement them untile version 5.<sup>4</sup> However, there are external (non-intrinsic) IEEE modules for gfortran on the x86 (support both 32 and 64 bit) that are included into the **HEDTOOLS** bundle.



# Important

the **fimm** HPC cluster, where calculations are normally performed, has GNU Fortran 4.8.1 and will require non-intrinsic IEEE modules. It also has the Intel Fortran which has built-in (intrinsic) IEEE modules though.

<sup>&</sup>lt;sup>4</sup> It was because GNU compiler collection is made for portability and supports many different processor architectures in addition to the most common x86 and implementation of IEEE modules is highly dependent on the CPU type and features.

# 12.2 IEEE Exceptions

There are several exception conditions:

- IEEE\_DIVIDE\_BY\_ZERO
- IEEE\_INEXACT
- IEEE INVALID
- IEEE OVERFLOW
- IEEE\_UNDERFLOW
- IEEE USUAL (An array of three exceptions IEEE OVERFLOW, IEEE DIVIDE BY ZERO, IEEE INVALID)
- IEEE\_ALL (An array of five exceptions IEEE\_OVERFLOW, IEEE\_DIVIDE\_BY\_ZERO, IEEE\_INVALID, IEEE\_UNDER FLOW, IEEE\_INEXACT)

Normally, if the program encounters invalid arithmetic calculations, then it should crash or at least report the problem. Otherwise, correctness of calculations is not guaranteed. By default, many compilers just **ignore** invalid calculations (even many cases of division by zero, NaN<sup>5</sup> generation etc.).

In most cases NaNs and other invalid arithmetics strongly point to a bug. If a NaN value is just left ignored during the calculations, it will likely propagate further into some other calculations making them invalid. It is therefore wise to turn halting ON by default in *model* calculations (unlike normal utility software that should never crash).

Turning arithmetic exception halting ON during the compile time requires specific compiler options.

Compiler	option	example
GNU GCC	-ffpe-trap	-ffpe-trap=zero,invalid,overflow,underflow
Intel Fortran	-fpe (/fpe)	-fpe0(/fpe:0 on Windows)
Solaris Studio	ftrap	ftrap=invalid,overflow,division

The IEEE module IEEE\_EXCEPTIONS allows to control halting during the run time. For example, it is cool to switch halting ON in specific troublesome parts of the code that can normally result in invalid calculations (division by zero, invalid, inexact etc.) and control each such occurrence specifically (e.g. provide a subroutine handling and fixing the calculations).

Halting the program that encounters specific condition is controlled via <code>IEEE\_GET\_HALTING\_MODE</code> subroutine (returns logical parameter <code>IEEE\_DEF\_MODE</code>). For example, for <code>IEEE\_INVALID</code> it is:

```
call IEEE_GET_HALTING_MODE(IEEE_INVALID, IEEE_DEF_MODE)
```

It is also possible to set specific halting mode for specific condition. For example, to set halting ON (execution termination) on invalid arithmetic do this:

```
call IEEE_SET_HALTING_MODE(IEEE_INVALID, .TRUE.) ! Will halt on IEEE_INVALID
```

Here is an example:

```
! Invoke IEEE Arithmetics:
! use, non_intrinsic :: IEEE_EXCEPTIONS ! if gfortran v<5
! We normally use included auto-generated wrapper for the module include "IEEE_wrap.inc"

IMPLICIT NONE

REAL  r,c,C0,Ap,Vc,Ke,Eb</pre>
```

<sup>&</sup>lt;sup>5</sup> "Not a Number," a wrong arithmetic value that is not equal to itself, can result from many math errors

```
REAL FR1, FR2, F1, FDER
. . . .
logical :: IEEE_MATH_FLAG, IEEE_DEF_MODE ! values for IEEE math modules
call IEEE_GET_HALTING_MODE(IEEE_INVALID, IEEE_DEF_MODE) ! Get default halting
call IEEE_SET_HALTING_MODE(IEEE_INVALID, .FALSE.)
                                                   ! NO halting from here!
FR2=LOG(ABS(C0)*Ap*Vc)
FR1=LOG(((Ke+Eb)/Eb)*r*r*EXP(c*r))
F1 = FR1-FR2
FDER = c + 2./r
call IEEE_GET_FLAG(IEEE_INVALID, IEEE_MATH_FLAG) ! Get the error flag
if (IEEE MATH FLAG) then
  ! if IEEE exception is signalled, we cannot relay on the calculations
  ! Report the error: remember there is no halting now, the program won't stop
 write(10,*) "IEEE exception in DERIV", r,F1,FDER,c,C0,Ap,Vc,Ke,Eb
  ! We also have to fix the calculations, e.g. equate some values to zero
 r=0.; F1=0.; FDER=0.
 call IEEE_SET_FLAG(IEEE_INVALID, .FALSE.) ! Set the error flag back to FALSE
end if
call IEEE_SET_HALTING_MODE(IEEE_INVALID, IEEE_DEF_MODE) ! Set default halting
END SUBROUTINE DERIV
```

# 12.3 Implementation details

We use an automatic build system (see below) which normally keeps track of the compiler and its version and IEEE modules support, there is no need to include use, intrinsic (or non\_intrinsic) ::IEEE\_EXCEPTIONS and tweak it manually depending on the compiler support. The build system automatically generates the correct include file IEEE\_wrap. inc which should be inserted into the code in place of use ... statement:

```
SUBROUTINE DERIV(r,F1,FDER,c,C0,Ap,Vc,Ke,Eb)
!Derivation of equation for visual range of a predator

! Invoke IEEE Arithmetics:
! use, non_intrinsic :: IEEE_EXCEPTIONS ! if gfortran v<5

! We normally use included auto-generated wrapper for the module include "IEEE_wrap.inc"

REAL r,c,C0,Ap,Vc,Ke,Eb
....
```

Without the GNU make-based build system, the rule is simple. Use **non-intrinsic** modules with GNU gfortran version <5.0 <sup>6</sup> and build the modules beforehand:

```
!**************
! *** NON-PORTABLE CODE BEGIN ***
use, non_intrinsic :: IEEE_FEATURES
use, non_intrinsic :: IEEE_ARITHMETIC
```

<sup>&</sup>lt;sup>6</sup> e.g. gfortran on the fimm cluster

and **intrinsic** modules on GNU gfortran v>5, Intel Fortran or Oracle Fortran:

# 13 Build system: GNU make

#### 13.1 Overview

The model currently uses a build system based on GNU make (Makefile). GNU make is an automated system for building source core (in fact, any digital project that requires keeping track of dependencies between multiple components.)

The make program is intended to automate the mundane aspects of transforming source code into an executable. The advantages of make over scripts is that you can specify the relationships between the elements of your program to make, and it knows through these relationships and timestamps exactly what steps need to be redone to produce the desired program each time. Using this information, make can also optimize the build process avoiding unnecessary steps.

— Mecklenburg R. Managing Projects with GNU Make

All the build rules for building the model executable are collected in the Makefile. If the model requires external components (e.g. non-intrinsic IEEE math modules), they will be automatically inserted.

GNU make is good because it works on diverse combinations of platforms and OSs (e.g. Linux and Windows). Some proprietary Unix platforms could supply the vendor's make utility that may not be compatible with the GNU make (e.g. Oracle Solaris includes its own make clone). There might be an option turning on GNU compatibility. But it is better to use the GNU make (gmake on Solaris) anyway.



#### **Important**

A good manual on the GNU Make is this book: Mecklenburg, R, 2005, *Managing Projects with GNU Make*, Third edition. O'Reilly. There is also the official GNU Make Manual.

# 13.2 Using make

Most basic things with the standard Makefile are simple. The commands are issued on the terminal console.

#### 13.2.1 Building and running the model

- Get a short help on the options: make help
- Autogenerate model documentation with Doxygen: make docs
- Build the model executable using default compiler: make
- Force rebuild the model executable with Intel compiler: make intel
- Force rebuild the model executable with GNU compiler: make gnu
- Run the current model: make run (on the fimm HPC cluster, this will automatically start a new batch job)

#### 13.2.2 Cleanup

There are also a few options for deteting the files and data generated by the build process.

- Remove all the data generated by the model make cleandata
- Remove all the data files generated by the model run as well as the model executable: make clean
- Remove everything generated by the build system and all the data, retain the default state: make distolean

#### 13.2.3 Debugging

The environment variable DEBUG controls whether the build system produces the debug symbols (-g) or, if NOT defined, speed-optimised machine code (-O3, automatic loop parallelization etc.). To build with debug support just define DEBUG in the manner standard for the platform/OS. For example, on Linux use:

```
$ DEBUG=1 make
```

or (DEBUG is now persistent)

```
$ export DEBUG=1
$ make
```

#### on Windows:

```
O:\WORK\MODEL\HED18>set DEBUG=1
O:\WORK\MODEL\HED18>make
```

or use DEBUG as a parameter to make, this works on all platforms:

```
$ make intel DEBUG=1
```

The make system keeps track of all the code components. For example, if only one has been changed, it will recompile only this. It also keeps track of whether IEEE math modules are really necessary and if the intrinsic or non-intrinsic modules are used.

For example, you may have built the model executable (make) and then edited the code of a module a little. Then just issue command to run batch (make run) on fimm. The make system will then automatically determine that the model executable is now out of date and recompile the changed module and build an updated executable, and only after this will start the batch job.

Another example: you just checked-out or updated (e.g. svn up) the model source that is tested and known to be bug-free on the fimm cluster. Now you should compile components of the program, (e.g. tweak IEEE math modules), build the executable, and finally start the executable in the cluster's batch job system. All this is done using a single command: make run.

```
$ svn update
$ ... some output...
$ make run
```

The system should work the same way on Windows and Linux, including the fimm HPC cluster. By editing the Makefile provided, one can easily tweak the behaviour of the build process, e.g. add other modules, change names, compilation options and details etc.

Microsoft Studio, Oracle Solaris Studio and other similar IDEs actually provide their own make systems (e.g. nmake, make or dmake) that work behind the scenes even if the IDE GUI is used.

#### 13.2.4 Using Intel Parallel Studio on Windows (command line)

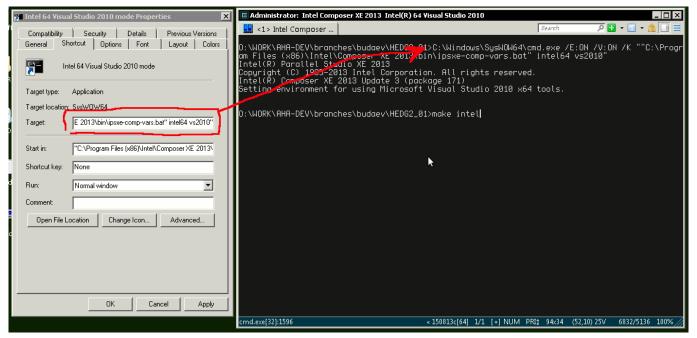
Using Makefile with the Intel Parallel Studio XE 2013 Fortran compiler (ifort.exe) (and probably other versions of Intel Fortran on Windows) requires setting up the Microsoft Studio environment. This is normally done by calling the Command Prompt from the menu:



Or if you right click on the shortcut, copy the commend line set in the menu and run it in the terminal. Such a command may look like this:

C:\Windows\SysWOW64\cmd.exe /E:ON /V:ON /K ""C:\Program Files (x86)\Intel\Composer XE 2013\ ← bin\ipsxe-comp-vars.bat" intel64 vs2010"

Then running this command will result in this:



Once the Intel command prompt environment is set, we can use the make command as normal with the Intel Fortran compiler, e.g. build using the Intel ifort on Windows:

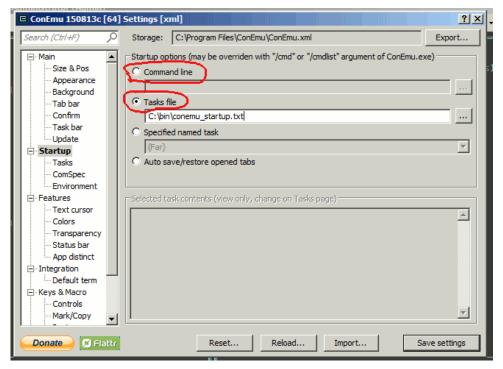
make intel



#### **Important**

It is crucial to set up the Intel Fortran command prompt build environment on the Windows platform, otherwise make would not find all the necessary Intel Parallel Studio and Microsoft Studio compiler and linker components. This is not necessary on the Linux Intel Fortran compiler.

If you use the ConEmu terminal, the command to set up the Intel Parallel Studio environment can be inserted in the ConEmu startup command line or script.

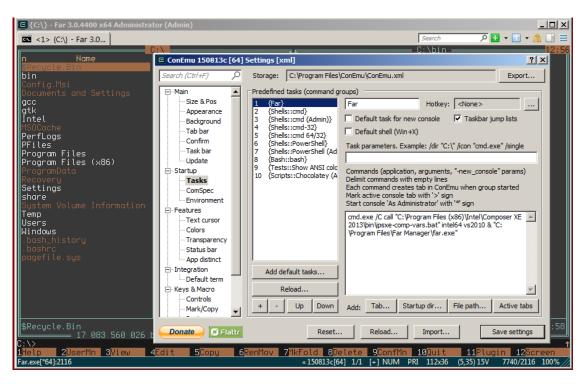


In the simplest case, the **Startup** command line or startup script might contain something like this (note that it is a single line with commands separated by ampersands &):

```
cmd.exe /C call "C:\Program Files (x86)\Intel\Composer XE 2013\bin\ipsxe-comp-vars.bat" \Leftarrow
intel64 vs2010 & "C:\Program Files\Far Manager\far.exe"
```

The exact path to the <code>ipsxe-comp-vars.bat</code> should be taken from the menu shortcut. In the above case, ConEmu will call the command prompt setup batch script <code>ipsxe-comp-vars.bat</code> (with full path and platform parameters <code>intel64 vs2010</code>) and then run the Far Manager (also full path is here).

If you like to use different **tasks** in ConEmu, such initialisation command, tweaked for particular task can be also inserted the **Startup**  $\rightarrow$  **Tasks**  $\rightarrow$  **Commands** menu; here is an almost identical example calling Far Manager:



Then, all the Intel build environment commands will be run automatically every time the ConEmu terminal is started (or the task is started), so you would not need to runt it manually.

# 13.3 Tweaking Makefile



# **Important**

In most cases only the model source code file(s) may need tweaking. This is defined in the variable SRC of the Makefile. Also, path to the Modelling tools, HEDTOOLSDIR, may need an update. Everything else should work out of the box.

# 13.3.1 Concepts

The two most important concepts for writing Makefile are **variables**, **macros**, **rules** and **targets**. In essence, Makefile just defines *rules* that build *targets* from their *prerequisites* using *variables* and *macros*.

Everything that starts from # is considered a comment.

**Variables** are defined as in shell scripts, for example:

```
# This variable defines the compiler command
GF_FC = gfortran
```

Variable can be *expanded*. The simplest kind of it is just assignment of a value from another variable:

```
# FC now gets value from GF_FC
FC = $(GF_FC)
```

A variable can get value from the output of the a shell script, then it should start from shell keyword, e.g.

```
# Check GCC version, it just calls: gfortran -dumpversion
# gfortran is obtained from the variable GF_FC
GFORTVERSION = $(shell $(GF_FC) -dumpversion)
```

There are also automatic variables, such as:

\$@ The filename representing the target, \$< The filename of the first prerequisite, \$? The names of all prerequisites that are newer than the target, separated by spaces,  $^{\circ}$  The filenames of all the prerequisites, separated by spaces,  $^{\circ}$  The filename of the target without suffix.

Macros are like multi-row variables that define a sequence of actions, a kind of "subroutine." For example, the following macro has the name AUTOGEN\_COMMENT, it uses the standard echo shell command and file redirection > to write (autogenerate) a piece of source code, the file name is defined by \$ (AUTOGEN\_HEADER):

This sequence of actions can be called just like a variable:

```
$ (AUTOGEN_COMMENT)
```

Targets define the file (e.g. executable program name) or other thing (e.g. some other target) that we are going to build. The line may also include prerequisites we need for compiling/building and finally the command(s) that actually do the build. In the simplest form a target with the name target\_0 can be written like this:

```
target_0: prerequisite_1 prerequisite_2
  commands
```

Then the make system checks that prerequisite\_1 and prerequisite\_2 do exist and are newer than the target (by the file modification time), and then rebuilds the target\_0 using commands. The system may go to other targets that are differed by the prerequisites to update them.



### **Important**

The commands that are defined to build a target in the Makefile (i.e. below the colon: part) must start from the TAB symbol.

For example, the part below has the target BASE\_UTILS.o (compiled object file), the prerequisite for compiling this file is Fortran source code BASE\_UTILS.f90, The system builds the target BASE\_UTILS.o using the compiler defined with \$ (FC) with compiler flags \$ (FFLAGS) -c, also here \$< is the first prerequisite, in this case the source code file (BASE\_UTILS.f90).

```
BASE_UTILS.o: BASE_UTILS.f90 $ (FC) $ (FFLAGS) -c $ <
```

If the system does not find the target file, it is compiled using the provided rule commands. Furthermore, if it finds out that we have already got the target file BASE\_UTILS.o but it is older than the source code BASE\_UTILS.f90 (the prerequisite), then this means that the target is "outdated" and should be re-compiled from the source.

A target may also be defined by a variable, e.g.

```
# Produce tweaked include file for PRNG
$(AUTOGEN_HEADER): $(BASE_RANDOM.f90) $(THIS_FILE)
$(AUTOGEN_COMMENT)
$(AUTOGEN_CODE)
```

The above code defines the rule to write the source include header file with the name defined by \$(AUTOGEN\_HEADER) with the prerequisites \$(BASE\_RANDOM.f90) and \$(THIS\_FILE) using the actions defined by the two macros (or variables): \$(AUTOGEN\_COMMENT) and \$(AUTOGEN\_CODE).

#### 13.3.2 Basic parameters

There are only few parameters in the Makefile that may need manual tweaking. The two variables that always need tweaking are, understandably, the file name(s) for the model code: SRC and the name of the executable OUT (although the latter may always be MODEL.exe).

The variable SRC defines **the main source code** file(s) for the model (HEDTOOLS are separate).

```
# These names should be set for particular project,
# Most probably they should be edited manually for each specific project
# SRC is the name of the main source code (can be several files). Note that
# Intel fortran doesn't like f95 file extension, use f90
# OUT is the executable file

SRC = HEDG2_03.f90

OUT = MODEL_00.exe
```

Several files of the model source code can be defined, e.g.

```
SRC = HEDG2_03.f90 HEDG2_03U1.f90 HEDG2_03U2.f90 HEDG2_03U3.f90
```

or wildcards for files in the current directory (or several wildcards) can be used:

```
SRC = HEDG2*.f90
```

The variable HEDTOOLSDIR defines the location of the source code for the **modelling tools/modules**. In most cases the file hierarchy is simple, model code and the HEDTOOLS code are in separate subdirectories.

In such a case, HEDTOOLSDIR is defined in the Makefile as follows:

```
# Path to HEDTOOLS and IEEE non-intrinsic libs
HEDTOOLSDIR = ../HEDTOOLS
IEEEPATH = $(HEDTOOLSDIR)/IEEE
```

Here are some of the variables that might need re-definition:

- FC is the default compiler,
- SRC is the source file name(s) for the model (almost always needed!),
- OUT is the executable name to be built,
- HOST\_HPC\_ROOT host name of the HPC cluster where the model is run by submitting the cluster job (normally fimm),
- HEDTOOLSDIR path to the modelling tools (HEDTOOLS),
- IEEEPATH path to the non-intrinsic IEEE modules (normally \$ (HEDTOOLSDIR) / IEEE),
- GF\_STATIC GNU compiler options for static build,
- GF\_TRAPS GNU compiler options for IEEE arithmetic traps,
- GF\_RCHECKS GNU compiler options defining runtime code checks,

- GF FFLAGS GNU compiler flags, optimisations etc.,
- IF\_ Intel compiler options with the same purposes as the above GF\_-flags.

The definition of the supported compilers and the **the default compiler** (that is used if make is called without parameters) is like this:

```
# Supported Fortran compiler types
GF_FC = gfortran
IF_FC = ifort
SF_FC = f95
# Choose the default compiler type
FC = $(GF_FC)
```

So, to tweak the Makefile to use the Intel compiler as default, just change this:

```
FC = \$(IF\_FC)
```



#### **Important**

The Makefile code is documented, just read the comments and explanations for the different variables and macros.

# 14 Using Microsoft Visual Studio

# 14.1 Working with the source code of the Modelling Tools

#### This is a difficult but flexible method.

Developing and debugging the code that uses the source code of the HEDTOOLS modelling tools with Microsoft Visual Studio on the Windows platform should follow such a workflow.

- 1. Create the model project in Microsoft Visual Studio as usual.
- 2. Include the source . £90 files from HEDTOOLS that are used in the project into the current Microsoft Studio project. Source files can be just copied into the model source code directory for convenience.
- 3. Manually **tweak** the source code for these non-portable modules, that make use of auto-generated include files in the make system. Currently, there are two such modules: BASE\_RANDOM and IEEE Modules
- 4. Compile/Build/Debug and work with the model code(s) as normal from within the Misrosoft Studio
- 5. The model code can be (re)built using the command line tools and the make-based system. Just do not forget to point to the location of the **original unedited** HEADTOOLS code within the Makefile. The Modelling tools code tweaked manually as a part of the Visual Studio Project cannot be used by the make system.

### 14.2 Building the Modelling Tools as a static library

#### This is the easiest method not requiring any manual tweaks.

An easier and more convenient way to include the HEDTOOLS modelling tools to a Microsoft Visual Studio / Intel Parallel Studio Project is to build the tools as a **static library** that is then included into the current model coding project. This method does not require manual tweaking of the modelling tools source code and takes full advantage of the automatic make system <sup>7</sup>. Also, the same library file can be included into many different Visual Studio projects. However, the tools library must be built using exactly the same platform and compiler.

<sup>&</sup>lt;sup>7</sup> Although, if IEEE Modules are used in the code, the code should be tweaked manually



# Important

Never mix static library produced with GNU fortran into Intel Parallel Studio projects or vice versa, or even different versions of Intel Parallel Studio Fortran—the library and the project code must be built using the same compiler.

First, build the HEDTOOLS modelling tools as a static library using the make system with FC=ifort, this is the default make target. Do not forget to make sure the Intel Parallel Studio **Command Prompt Environment** has been correctly prepared prior to the build process.

make FC=ifort

On the Windows platform with Intel Fortran compiler, this will produce a static library file with this name: **lib\_hedutils.lib** as well as many **.mod** header files. For convenience, the make system also produces a **zip** archive containing all the re-distributable tool files.

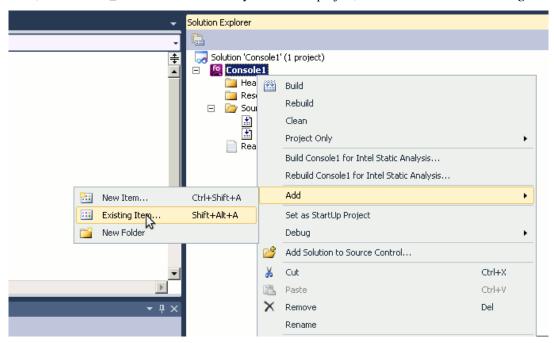


#### **Important**

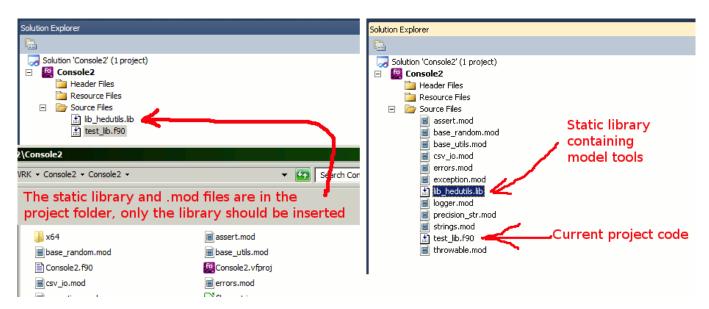
The Makefile producing the library requires two command line GNU utilities: uname and zip. Windows versions are available from GnuWin32 and other distributions. If these utilities are not available, the static library is still produced although the handy **zip** file distribution is not generated.

First, copy .mod files to the current Visual Studio Project folder containing the source code .f90 files. The library itself should be also placed there. It is convenient to just unzip the whole content of the redistributable **zip** file created by the make system.

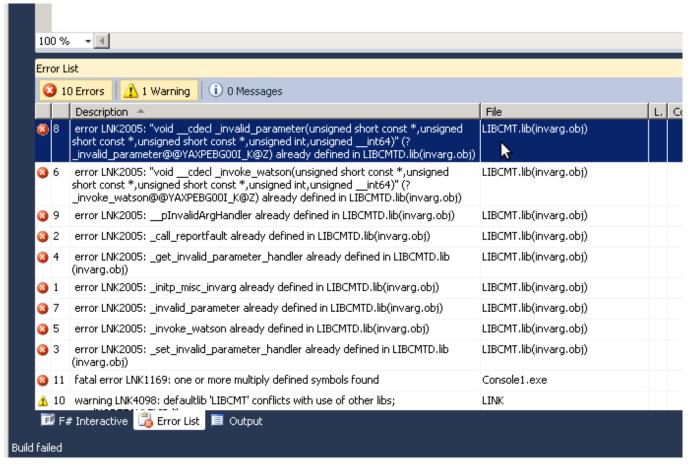
Then, insert the **lib\_hedutils.lib** static library file into the project, use the menu  $Add \rightarrow Existing Item$  menu.



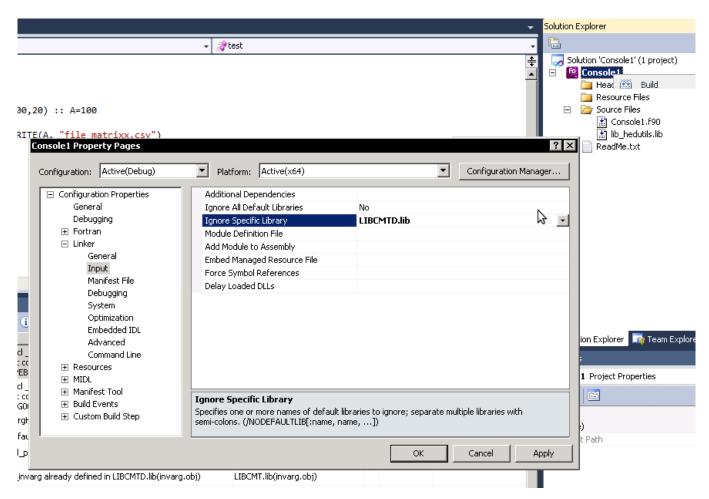
It is also possible to add the library into the project directly from the HEDTOOLS directory, in such case, also add all the .mod from HEDTOOLS to the project. Then, the library and .mod files are accessed directly from the Modelling Tools folder and should not be copied to the current project folder and can be included from their own directory to several Visual Studio projects.



Now the code should build successfully (calling the modelling tools code from the library) as normal (e.g.  $Build \rightarrow Build$  Solution). There may be problem with the LIBCMTD.lib library in the Debug solution (I have not encountered the same issue in the Release solution though):



If there is such a problem, go to **Properties**  $\rightarrow$  **Linker**  $\rightarrow$  **Input** and insert the problem library LIBCMTD.lib to the **Ignore Specific Library** field:



From now, it should (hopefully) build without further issues. The modelling tools are now automatically inserted by the compiler into the executable code from the static library provided as if the subroutines and functions were intrinsic.

### Using the static library tools for command line building

Finally, if you like to build code with the static library from the command prompt rather than Visual Studio IDE, it is also easy:

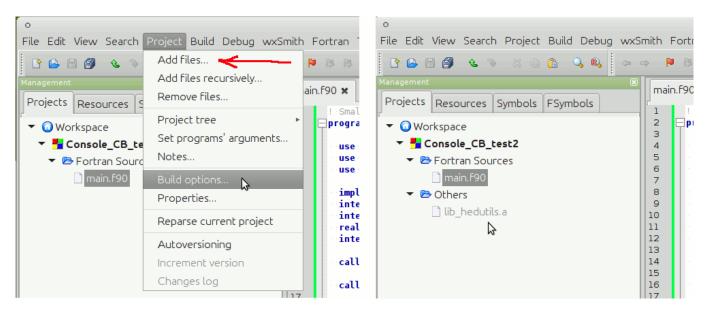
```
ifort file.f90 lib_hedutils.lib
```

This command compiles and links the code in file.f90 with the library.

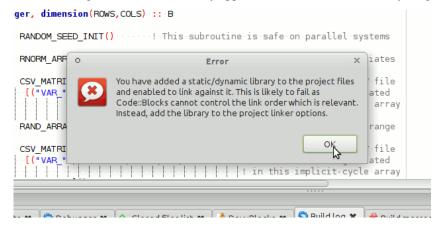
The static library can be built on any of the supported platforms (Windows, Linux, Mac) and compilers (e.g. GNU gfortra and Intel Fortran). But note that on Unix systems and GNU gfortran on Windows the library has an .a rather than .lib file extension. The redistributable **zip** file that is produced when building the library contains a small Readme.txt file.

# 15 Using Code::Blocks IDE

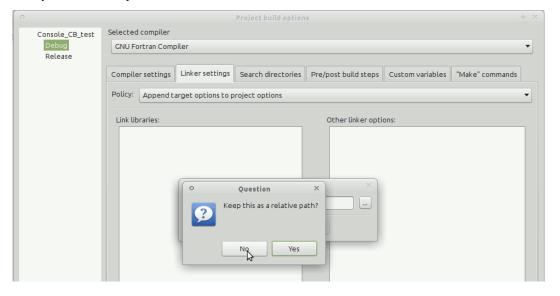
Working with the Code::Blocks IDE is similar to that with Microsoft Studio. The simplest way to get it running is to (1) build HEDTOOLS as a static library using the make system, (2) copy the library file lib\_hedutils.a (or lib\_hedutils.lib) and all the .mod files produced by the make build system into the working project directory, add the library file to the project file using the **Project**  $\rightarrow$  **Add Files** menu. After this it should build within the IDE.



When building, a link order issue may appear, but this does not affect anything, so in most cases just ignore it.



Alternatively, the library can be inserted using the  $\mathbf{Project} \to \mathbf{Build\ Options} \to \mathbf{Linker\ settings}$ . Using this method, you might get an issue with the compiler not being able to find the library (as it is not in the LIBPATH). Not keeping relative path to the library will solve the problem.



# 16 Manual builds of HEDTOOLS

# 16.1 Editing source codes

If the model is built *without* using the automatic GNU make utility and the supplied Makefile, you should take care about the dependencies and header files yourself. These are the modules that require manual source tweaking in such cases:

- BASE\_RANDOM
- IEEE Modules

These pieces of code should be edited manually depending on the compiler and its version used. Please check your documentation. Make sure all source code files for the model as well as for the HEDTOOLS are included in the project. Many IDEs allow generating (importing) project from a supplied Makefile and recognize GNU make format. This could make work a little easier.

# 16.2 Using static library

Another option is (1) to build the **modelling tools** as a static library using the make system. (2) Compile the model and link the tools in from the library. Then, no manual edits may be required. Refer to the Readme.txt file that is produced with the static library. When using the Intel Fortran compiler on Windows, make sure the command prompt environment is correstly set up.

This is a small test program code producing two random matrices and saving them to CSV:

```
! test_lib.f90 :: Small test of the HEDTOOLS
program test_library
 use CSV IO
                  ! we use these modules
 use BASE UTILS
                  ! from HEDTOOLS
 use BASE_RANDOM
 implicit none
 integer, parameter :: ROWS=1000, COLS=20
 integer :: i
  real, dimension (ROWS, COLS)
 integer, dimension(ROWS,COLS) :: B
  call RANDOM_SEED_INIT()
                          ! This subroutine is safe on parallel systems
  call RNORM_ARRAY(A)
                                 ! Generate a matrix of random normal variates
  call CSV_MATRIX_WRITE(A, "file_matrix_a.csv",& ! Save the matrix to CSV file
        [("VAR_" // TOSTR(i, COLS), i=1, COLS)])
                                                ! Column names are generated
                                                 ! in this implicit-cycle array
 call RAND_ARRAY(B, 10, 100)
                           ! Generate a random integer matrix with range
  call CSV_MATRIX_WRITE(B, "file_matrix_b.csv",& ! Save the matrix to CSV file
        [("VAR_" // TOSTR(i,COLS),i=1,COLS)])
                                              ! Column names are generated
                                                 ! in this implicit-cycle array
end program test_library
```

End of the document.

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