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 approach 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/branches/budaev/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)

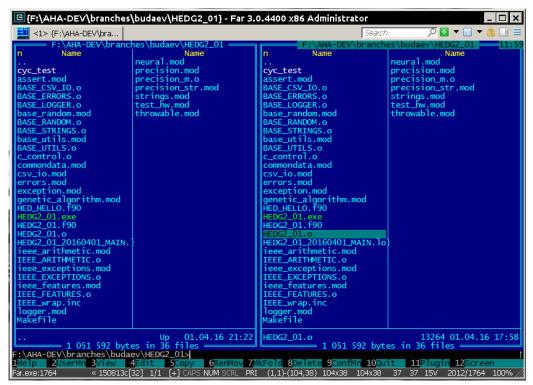
Intel Fortran compiler, a commercial software available at UiB. Intel Fortran is also installed on the UiB HPC cluster fimm. Free GNU Fortran distribution along with make and other tools is available from the Equation solution http://www.equation.com/servlet/equation.cmd?fa=fortran. There is also Oracle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

Subversion (Mandatory)

Windows GUI for Subversion is **TortoiseSVN** (supported by UiB IT): https://tortoisesvn.net/. It is very helpful to have also console subversion client software (Tortiuse includes console tools but does not install by default). A good one is SilkSVN https://sliksvn.com/download/.

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 http://doxygen.org/. On Windows is is also highly desirable

to have a LaTeX distribution, such as MikTeX (http://miktex.org) and Ghostscript (http://www.ghostscript.com), both are free software. LaTeX and Ghostscript are required to generate PDF.

Geany (Recommended)

Lightweight IDE, Editor for code and any text files. Works on Linux, Windows and Mac. http://www.geany.org/ Also need plugins: http://plugins.geany.org/

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.

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

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.

Use meaningful labels

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:

```
realgen = realgen +1
end do GENERATIONS_LOOP
```

```
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, as well as built-in 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 (-03 -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.

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 using the above tricks that works fast just everywhere.

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 doxywizerd 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:

```
!-----
!> @brief Module **COMMONDATA** is used for definine various global
!! parameters like model name, tags, population size etc.
!! @details Everything that has global scope and should be passed to many
!! subroutines/functions, should be defined in 'COMMONDATA'.
!! It is also safe to include public keyword to declarations.
!! '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
```

¹ 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

```
!! 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
```

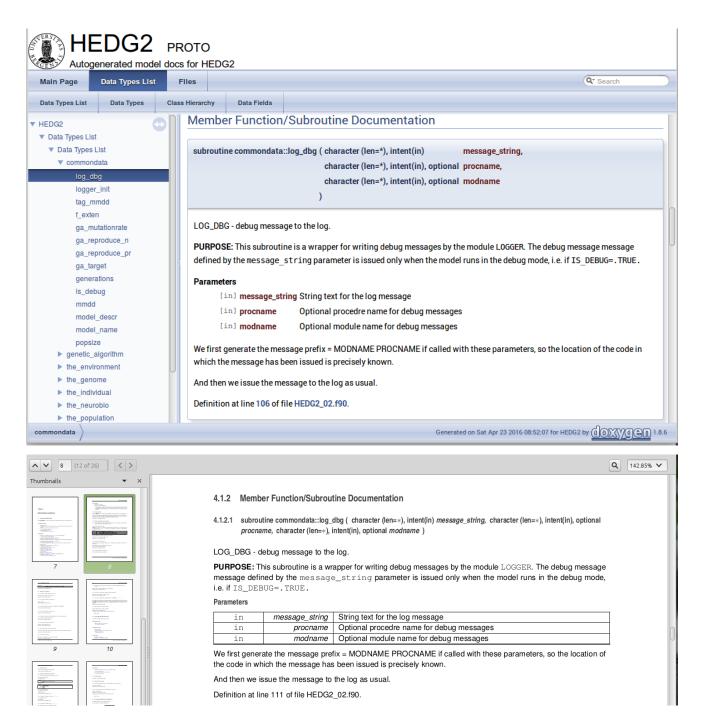
@brief starts a paragraph that serves as a brief description. @details starts the detailed description.

@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.).

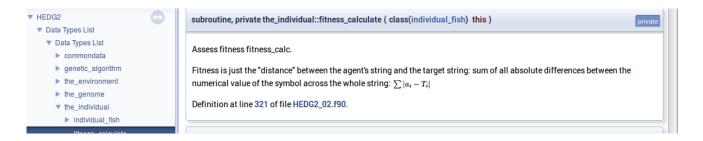
There are different options to generate HTML documents. For example, a bundle of HTML files with images, cross-references, code syntax highlighting and search functionality can be prepared. Alternatively, a single simpler HTML file can be done. LaTex output can be converted to PDF with references and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

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

4 Version control: Subversion (SVN)

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

4.1 Overview

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.

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 yoi 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:

4.2 First time setup of the working copy

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. For example, first time checkout (for user u01):

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

```
Terminal - mc [budaev@BIO195148]:~/Downloads — + > Tile Edit View Terminal Tabs Help

budaev@BIO195148 ~/Downloads/zzz $ svn -- username = checkout https://svn.uib.no/aha-fortran

Authentication realm: <a href="https://svn.uib.no:443">https://svn.uib.no:443</a>> UiB SVN Repository

Password for 's 2'://*********

ABC

Hei,
```

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.

```
0
                         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
```

4.3 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...
- commit, when ready (e.g. when a new 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"
```

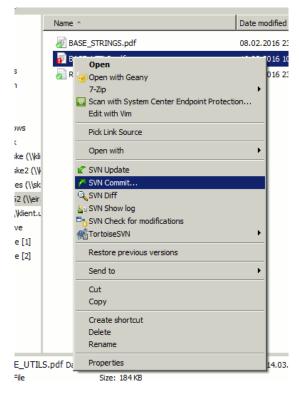
Both update and commit can be done for the working directory as well as for specific file. E.g. to commit only the model code Hed18.f90 do:

```
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.

4.4 GUI Tools

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



Similar GUI tools exist for Linux. For example, there is thunar-vcs-plugin (Git and subversion integration into the Thunar file manager).



4.5 Some Recipes

Here are a couple of recipes for certain less obvious SVN commands that are not a part of standard everyday workflow but used nevertheless from time to time.

4.5.1 Make a branch

Yet not done, will do when I next time do branching:) Shall just copy real commands and paste them here.

4.5.2 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 syncronised.

```
# First, make sure you are in the branch .../branches/budaev/HEDTOOLS
pwd

# 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
# If everything is in order, do the real merge:
svn merge ^/trunk/HEDTOOLS/
```

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
```

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').

```
module THE_GENOME
                                             ! The module defines GENOME object
. . . .
type, public :: INDIVIDUAL_GENOME
                                             ! It is defined here
 character(len=len(GA_TARGET)) :: str
                                                we have user (derived) type
  contains
                                                 ... and type-bound procedures.
   procedure, public :: init_genome => init_genome_random
   procedure, public :: mutate => mutate_genome
end type INDIVIDUAL_GENOME
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
                                             ! the left of "=>"
contains
  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

end module THE_NEUROBIO
```

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 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)²

```
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:

```
print *, ">>", TOSTR(3.1415926,"(f4.2)"), "<<"
produces >>3.14<</pre>
```

```
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>
```

² Note that float point calculations, especially single precision (real type 4) may introduce a rounding error

```
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:

```
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 0.500000000 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>
```

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:

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

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).

Example

```
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.

The typical workflow for output in CSV file format is like this:

- CSV_OPEN_WRITE physically open CSV file for writing;
- CSV_HEADER_WRITE physically write optional descriptive header (header is just the first line of the CSV file);
- do start loop (1) over records (rows of data file)
 - do start loop (2) over values within the same record

CSV_RECORD_APPEND - produce record of data values of different types, append single values, arrays or lists, usually in loop(s)

end do — end loop (2)

CSV_RECORD_WRITE - physically write the current record of data to the output file.

- end do—end loop (1)—go to producing the next record;
- CSV_CLOSE physically closes the output CSV file.

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 1=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
```

Example

```
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:



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

Example

```
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.

Example

```
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_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."
```

8.11 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."
```

8.12 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.

8.13 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.

8.13.1 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)³ can be saved into CSV files using array slices, for example:

8.13.2 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**.

Example

 $^{^3}$ CSV_IO code could be modified to save higher-rank arrays if this function is needed

```
! 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):

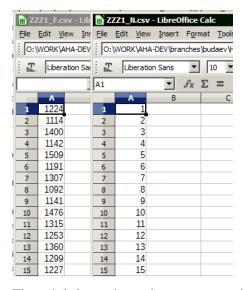
```
real, dimension(1:100,1:20) :: MatrixX   ! Matrix, two dimensional
real, dimension(1:100) :: Array_Y   ! Array, one-dimensional
......
call CSV_MATRIX_WRITE(MatrixX, "file_matrixx.csv")   ! write 2-d matrix
call CSV_MATRIX_WRITE(Array_Y, "file_array_y.csv")   ! write 1-d array
```

8.13.3 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.

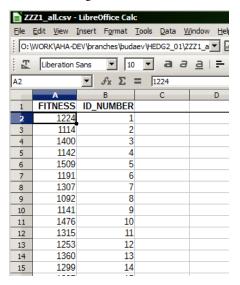
Suppose we have two integer object vectors generation_one%individual%fitness and generation_one%individual%person_number each having POPSIZE elements (these are just two one-dimensional vector components of a single object). Each of these vectors can be saved using the standard CSV_MATRIX_WRITE call:

```
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.

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.

8.14 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).

8.14.1 Basic Example

8.14.2 Arrays of structures

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

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 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 RAND I

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

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

9.3 RAND_R4 and RAND_R8

Generates a random real (type 4 or 8). Has no parameters.

```
if ( RAND_R4() < ga_mutationrate ) then
  call mutate(fish(i))
end if</pre>
```

9.4 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

```
!**************************
! *** NON-PORTABLE CODE BEGIN ***

! External Modules not used on Oracle f95, but an include header must be placed
implicit none

integer, allocatable :: seed(:)
integer :: i, n, un, istat, dt(8), pid
integer, parameter :: int64 = selected_int_kind(18) ! define int64
integer(int64) :: t
```

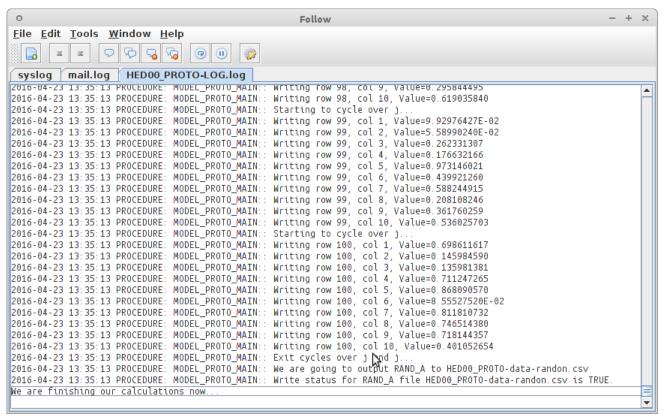
The build system based on GNU make does this automatically.

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 volume
level_string_chapter	string delimiter	Set the string for chapter
level_string_section	string delimiter	Set the string for section
level_string_subsection	string delimiter	Set the string for subsection

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:

```
call LOG_DELIMITER(1)     ! issues volume "-----"
call LOG_DELIMITER(LOG_LEVEL_SUBSECTION) ! issues subsection "+++++++++++"
```

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 http://www.gbenthien.net/strings/index.html. 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 http://www.gbenthien.net/strings/index.html. 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 arg2 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 5.⁴ 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.

⁴ 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, NaN⁵ 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>
```

⁵ "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 ⁶ and build the modules beforehand:

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

⁶ 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.

13.2 Using make

Most basic things with the standard Makefile are simple.

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.

13.3 Tweaking Makefile

13.3.1 Basic parameters

Here go basic parameters of the Makefile

13.3.2 Build options

Here build variables will be placed.



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.

14 Final Notes

Nothing so far...

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