Modelling Tools Manual

REVISION HISTORY

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Contents

Abstract

This document describes the modelling tools used for the new model environment. It is partly autogenerated. Autogeneration is incomplete at this time as most of the model components (actual for 2016-02-11).

SVN address of this document source is:
$HeadURL: https://svn.uib.no/aha-fortran/branches/budaev/HEDTOOLS/BASE_UTILS.adoc $

SVN date: $LastChangedDate: 2016-02-11 22:47:54 +0100 (Thu, 11 Feb 2016) $

1 Introduction

These modelling tools include two separate modules: **BASE_UTILS** and **CSV_IO**. 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.

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

```
program TEST

  use BASE_UTILS  ! Invoke the modules
  use CSV_IO      ! into this program

  implicit none

  character (len=255) :: REC
  integer :: i
  real, dimension(6) :: RARR = [0.1,0.2,0.3,0.4,0.5,0.6]
  character (len=4), dimension(6) :: STARR=["a1","a2","a3","a4","a5","a6"]

..........

end program TEST
```

Building the program with these modules using the command line is notmally 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.

2 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**.

2.1 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)

2.1.1 Examples:

Integer:

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

Single precision real (type 4)[1]

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

Double precision real (type 8)

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

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<<
```

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

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<<
```

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

```
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<<
```

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<<
```

[1] 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<<
```

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<<
```

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<<
```

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"
else
  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
```

```
string104 = "HED24-" // trim(MMDD) // trim(runtag) // "-E0" // &
            TOSTR(expmt,10) // "-o104-genepool-" // &
            "gen-" // TOSTR(gen, 10000000) //  "-" // &
            "age-" // TOSTR(age, 10000) // f_exten
```

2.2 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).

2.3 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<<
```

2.4 Subroutine: RANDOM_SEED_INIT

RANDOM_SEED_INIT is called without parameters and just initialises the random seed for the Fortran random number generator.

Example

```
call RANDOM_SEED_INIT
```

3 Module: CSV_IO

3.1 Overview

This module contains subroutines and functions for outputting numerical data to the CSV (Comma Separated Values) format (RFC4180, CSV format).

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 could be called irrespective of the order using named parameters, e.g. this way (the first optional parameter absent):

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

or (both parameters present but swapped in order):

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

or (optional parameters absent altogether):

```
intNextunit = GET_FREE_FUNIT()
```

or the standard way:

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

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 names for the header
record_csv="" ! but first, prepare empty record string
call CSV_RECORD_APPEND(record_csv,["VAR_001", ("VAR_" // TOSTR(i,100),i=2,Cdip)])
........
! 5. Now we can write records containing actual data values, we do this
!    in two do-cycles
CYCLE_OVER_RECORDS: do l=1, Cdip
  ! 6. Prepare an empty string for the current CSV record
  record_csv=""
  CYCLE_WITHIN_RECORD: do m=1, CNRcomp
    ....
    ! do some calculations...
    .....
    ! 7. append the next value (single number) to the current record
    call CSV_RECORD_APPEND ( record_csv, genomeNR(l,m) )
    .....
  end do CYCLE_WITHIN_RECORD
  ! 8. 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
! 9. 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
```

3.2 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
```

3.3 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

```
type(csv_file) :: file_occ          ! declare file handle object
........
call CSV_CLOSE(file_occ)            ! use file handle object
........
call CSV_CLOSE(csv_file_name=file_name_data1, &   ! old style
               csv_file_status=fstat_csv)
 if (.not. fstat_csv) goto 1000
```

3.4 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`

```
character (len=*) :: header          ! mandatory CSV file header
type(csv_file) :: csv_file_handle    ! file handle object
```

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.

3.5 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):

```
integer :: csv_file_unit               ! unit associated with open file name
```

Example

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

3.6 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:

```
logical :: file_status                 ! operation success status
integer :: max_funit                   ! maximum unit to search
```

Output parameter (function value):

```
integer :: file_unit                   ! the first free/available file unit
```

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()
```

3.7 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:

```
integer :: file_unit                  ! Fortran file unit to check
```

Output parameter (function value):

```
logical :: file_status                ! gets TRUE if the unit is valid
```

Example

```
if (.not. CHECK_UNIT_VALID(csv_file_unit)) then
      csv_file_unit=GET_FREE_FUNIT(csv_file_status, MAX_UNIT)
.........
```

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

3.8 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.

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.

3.8.1 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
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"])
```

3.9 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."
```

3.10 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:

```
character (len=*) :: csv_file_name        ! file name
integer :: csv_file_unit                  ! file unit
character (len=*)  :: record              ! current CSV record (mandatory)
logical :: csv_file_status                ! optional operation status, TRUE if
                                          !  success
```

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`

```
character (len=*)  :: record              ! current CSV record (mandatory)
type(csv_file) :: csv_file_handle         ! file handle object
```

Example

```
call CSV_RECORD_WRITE(csv_record, file_cop)               ! write current record
call LOG_MSG("Physically wrote record " // TOSTR(a) // &  ! report this in some
             " to the file " // file_cop%name // &        ! logging subroutine.
             ", write status =" // TOSTR(file_cop%status))
```

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

3.11 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 ina single code instruction.

It gets three parameters: one-dimensional array or two-dimensional data matrix (of any supported type), string file name and an optional logical file operation status.

```
integer, dimension(:,:) :: matrix     ! data object, array or 2-d matrix
character (len=*) :: csv_file_name    ! file name for output
logical :: csv_file_status            ! operation status, TRUE if success
```

There is also an alias to this subroutine, `CSV_ARRAY_WRITE`, which is for output of one-dimensional array to CSV.

Important
Note, that one-dimensional array is written to the file as a single row, not as a column.

Example

```
call CSV_MATRIX_WRITE (ARRAY_Z, "test-file-001.csv", fstat_csv)
 if (.not. fstat_csv) goto 1000
```

3.12 Derived type: csv_file

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

```
type, public :: csv_file
  character (len=MAX_FILENAME) :: name  ! The name of the file
  integer :: unit = -1                  ! Fortran unit associated with the file
  logical :: status = .TRUE.            ! success flag for the latest operation
end type csv_file
```

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`).

Example

```
type(csv_file) :: file_occ              ! define the file handle object
....
file_occ%name="some_name.txt"           ! set file name value
....
call CSV_OPEN_WRITE(file_occ)           ! Open file for writing
....
call CSV_CLOSE(file_occ)                ! Close file
```

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 Fortran (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.

4 Final Notes

There are a few other modules. I will write similar documentation for them too... Hope it is soon. There is still much to to.

The manual is generated with AsciiDoc markup processor. Later, an auto-generation of docs from the model code is planned (not first priority though).

5 Index