Computer Physics Communications 58 (1990) 119–125
North-Holland

MERLIN-2.1 DOUBLE PRECISION

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Received 8 August 1989

MERLIN-2.1 is an adaptation of the MERLIN-2.0 package, mainly designed to run on computers using 32-bit floating point arithmetic. The standard Merlin-2.0 on such machines, achieves a precision of 7 significant digits at most. This is insufficient since in many real problems a higher precision is required. MERLIN-2.1 treats this inadequacy using double precision operations, enhancing so the precision up to about 14 significant digits, in the standard user-friendly Merlin environment.

ADAPTATION SUMMARY

Title of adaptation: MERLIN-2.1 DOUBLE PRECISION

Adaption number: 0001

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland (see application form in this issue)

Reference to original program: *Title*: MERLIN-2.0 – enhanced and programmable version; *Cat.no*: ABHB; *Ref. in CPC*: 52 (1989) 241

Authors of original program: D.G. Papageorgiou, C.S. Chassapis and I.E. Lagaris

Computer for which the adaptation is designed and others on which it is operable: the adaptation is mainly designed for computers using 32-bit floating point numbers, but it will work on any machine equally well, since all changes are in ANSI Fortran 77

Computer: VAX 8350; *Installation*: INFN, Sezione di Pisa, University of Pisa, Italy

Operating system: VMS 5.1

High speed storage required: depending upon the maximum number of variables the object can handle (47000 words for 30 variables, 90000 words for 150 variables).

No. of bits in a word: 32

No. of lines required to effect adaptation: not applicable; a new source code is provided with a total of 7502 lines

Nature of physical problem
A lot of problems in physics, chemistry, applied mathematics as well as in engineering and in other fields, are quite often reduced to minimizing a function of several variables. MERLIN-2.1 is a programmable system designed to minimize a multi-dimensional function.

Method of solution
Six algorithms are implemented. Three of them make use of the function's gradient and hence are suitable for minimizing differentiable functions, the other three do not use derivatives at all and so are applicable to non-differentiable functions as well [2].

Reasons for the adaptation
The insufficient precision (7 significant digits) obtained when running on computers with a word of about 32 bits.

Restrictions on the complexity of the problem
Currently MERLIN is dimensioned to handle up to 150 variables. However, by redimensioning a few arrays it can easily be enhanced or reduced according to the user's needs, as described in the provided manual of the original program.

Typical running time
Heavily depending on the complexity of the objective function. Note that since all the calculations use double precision arithmetic, this version of the program is slower than the original release [1,2]. The test run took 6.30 cpu seconds on a VAX 8350 under VMS 5.1.

References

[1] D.G. Papageorgiou, C.S. Chassapis and I.E. Lagaris, Comput. Phys. Commun. 52 (1989) 241.
[2] G.A. Evangelakis, J.P. Rizos, I.E. Lagaris and I.N. Demetropoulos, Comput. Phys. Commun. 46 (1987) 401.

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LONG WRITE-UP

1. Introduction

MERLIN is an optimization package, that has been proved very effective in lots of problems, in physics, chemistry, engineering, etc. Both, its original release [1] and the programmable version [2], are written in ANSI Fortran 77, using single precision arithmetic. When using the program in a computer with 32-bit floating point numbers, the seven significant digits offered, may prove insufficient in some cases where increased precision is required. This version of the program cures the problem, offering double precision operations. Note that, since this version is also written in ANSI Fortran 77, one may use it in a computer with 64-bit floating point numbers, to increase the number of significant digits to about 28.

2. Detailed description

The following paragraphs describe the changes made to the program of ref. [2] and discuss how the user written part (FUNMIN, GRANAL, MASTER) should be. It is assumed that the reader is familiar with the MERLIN package as described in refs. [1,2].

2.1. Double precision variables

In order to achieve increased accuracy, we converted all single precision variables to double precision. This was done by means of the following implicit statement that was added in almost every subprogram:

```
IMPLICIT DOUBLE PRECISION (A-H,O-Z)
```

In addition we replaced all intrinsic functions with their generic names and all function subprograms were declared as DOUBLE PRECISION functions. We also converted every real constant to the D-exponent representation. E.g 5.0 is now written as 5.0D0.

2.2. The objective function FUNMIN

The user written objective function, namely FUNMIN, should be in double precision. There is no point having the program to operate in double precision, while FUNMIN performs the function evaluation in single. A typical FUNMIN declaration should be like:

```
DOUBLE PRECISION FUNCTION FUNMIN
(X,N)
IMPLICIT DOUBLE PRECISION (A-H,O-Z)
DIMENSION X(N)
```

2.3. Derivative calculation by GRANAL

If you decide to use your own derivative code, you must supply the GRANAL subroutine as described in ref. [1]. All the derivatives should be calculated using double precision. A typical GRANAL declaration should be like:

```
SUBROUTINE GRANAL(N,X,VAL,GRAD)
IMPLICIT DOUBLE PRECISION(A-H,O-Z)
DIMENSION X(N),GRAD(N)
```

2.4. The main program

MERLIN is called as a subroutine, and the user may want to write his own main program to do this. The call now involves double precision variables and should be of the form:

```
PARAMETER (NMAX = 30, NMAXW =
NMAX**2 + NMAX)
DOUBLE PRECISION VERSIM(NMAXW)
...
CALL MERLIN(N,VERSIM,NMAXW,IQUIT)
```

2.5. The input–output units

The unit numbers assigned to the standard input and output (defined in the Block Data EQUIP) have been set to 5 and 6, correspondingly; these unit numbers are used by many machines for interactive I/O. To run the program in batch mode, just change these values to the desired ones, or use the appropriate operating system command to assign these units to your input/output files.

2.6. The random number generator

The random number generator (used in subroutine RANDOM) is the only non-standard part of the program and will work only in VAX/VMS machines. You should replace the call to RAN with your local random number generator. The value returned must be uniformly distributed in (0,1).

2.7. The macro editor

MEDIT, the macro editor has been modified. No command other than E (Exit) and I (Insert) is allowed when the macro file is empty. (See the Merlin User's guide of ref. [1]) When using MEDIT to modify a line of the macro file, the incorrect line is printed on the screen and the user enters modification characters, below. These characters are input from the terminal, by a Fortran READ statement. This process has been proved to be non-portable, since some systems issue a prompt when reading data from a terminal, while others do not. A parameter (named INDENT) has been added to SUBROUTINE MODIFY, to control the positioning of the incorrect line during the modification process. You must set this parameter to the number of characters printed on the screen as prompt, by your local system. Currently this parameter is set to 0, implying that no prompt is printed during a Fortran READ.

2.8. A note on MCL

MCL is the programming language developed to drive MERLIN and help the user construct efficient minimization strategies [3]. The new version, MERLIN-2.1 presented here, is absolutely compatible with the object code generated by the MCL compiler. (The compiler itself does not need to be modified to handle double precision operations)

2.9. Other improvements

Several parts of the program have been improved in order to make it respond in a more friendly manner. Subroutine CHANGE has been modified to handle blank lines and incorrect input indices in a better way. Function FACT is now

Table 1
Objective function

```
      DOUBLE PRECISION FUNCTION FUNMIN(X,N)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION X(N)
      X1=X(1)
      X2=X(2)
      X3=X(3)
      FUNMIN=(X1-3)**2+5*X2**2*(X3-X1)**4+10*X3**2*(100-X1*X3)**2
      RETURN
      END

      SUBROUTINE GRANAL (N,X,VAL,GRAD)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION X(N),GRAD(N)
      X1=X(1)
      X2=X(2)
      X3=X(3)
      GRAD(1)=2*(X1-3)-20*X2**2*(X3-X1)**3-20*X3**3*(100-X1*X3)
      GRAD(2)=10*X2*(X3-X1)**4
      GRAD(3)=20*X2**2*(X3-X1)**3+20*X3*(100-X1*X3)**2
     >            -20*X3**2*X1*(100-X1*X3)
      RETURN
      END
```

written so as to allow factorials to be calculated within the accuracy of the particular machine. A parameter (which currently is set to 100, but may assumed any desired value) controls the range of the factorials. Subroutine DETUNT will now consider only units numbers in between 1 and 99.

3. Test run description

The objective function (listed in table 1) is the same as in refs. [1,2], written, however, in double precision. The input deck should reside in file FOR005.DAT, while the output is contained in the file FOR006.DAT. The test run took 6.30 CPU seconds on a VAX 8350.

References

[1] D.G. Papageorgiou, C.S. Chassapis and I.E. Lagaris, Comput. Phys. Commun. 52 (1989) 241.
[2] G.A. Evangelakis, J.P. Rizos, I.E. Lagaris and I.N. Demetropoulos, Comput. Phys. Commun. 46 (1987) 401.
[3] C.S. Chassapis, D.G. Papageorgiou and I.E. Lagaris, Comput. Phys. Commun. 52 (1989) 223.

TEST RUN INPUT

```
3
IAF
POINT
1  30  2  30  3  33.88
0
GODFATHER
X
Y
Z
SHORTDIS
ROLL
5  0  1  800  2  0
SHORTDIS
SIMPLEX
5  2000  6  0
SHORTDIS
BFGS
1  2000  6  0
DFP
 1  2000  6  0
SHORTDIS
STOP
```

TEST RUN OUTPUT

```
ENTER * OF VARIABLES
    -----------------------------------------------------------------------

   ............................        MERLIN-2.1 DOUBLE PRECISION VERSION
   ...........................                    ADAPTED BY :
   ...........................         D.G. PAPAGEORGIOU &   I.E. LAGARIS
   ...........................                PHYSICS DEPARTMENT
   ...........................               UNIVERSITY OF IOANNINA
   ...........................                   P.O.BOX 1186
   ...........................            IOANNINA - G R E E C E , 45110

   M E R L I N   2.1   (DOUBLE PRECISION)
   IOANNINA,   AUGUST - 1989
    -----------------------------------------------------------------------
   TO OBTAIN ON-LINE INFORMATION, MAKE SURE THAT
                          FILE:  HELP  , IS PRESENT
    -----------------------------------------------------------------------
ESTIMATED MACHINE'S ACCURACY:  0.10E-14

---------------------------------------------------------------------------
  ... ENTER PROCESSING MODE OPTION. ( BATCH / IAF )

---------------------------------------------------------------------------


   ....    W A R N I N G    ....
  ...   INITIALIZE VARIABLES   ...


      /\/\/\/\/\/\       MERLIN    IS AT YOUR COMMAND !!!
  POINT
  POINT


      /\/\/\/\/\/\       MERLIN    IS AT YOUR COMMAND !!!
  GODFATHER
 VARIABLE              1   :
 VARIABLE              2   :
 VARIABLE              3   :
             1) .... X
             2) .... Y
             3) .... Z
```

```
     /\/\/\/\/\/\       MERLIN    IS AT YOUR COMMAND !!!
 SHORTDIS
 TOTAL NU. OF CALLS =               1
 NU. OF CALLS SINCE LAST RESET                1
    1) X            .......   30.000000000000
    2) Y            .......   30.000000000000
    3) Z            .......   33.880000000000
          VALUE.......        9639759228.5377


     /\/\/\/\/\/\       MERLIN    IS AT YOUR COMMAND !!!
ROLL
--------------------------------------------------------------------------
                               ROLL - PANEL
--------------------------------------------------------------------------
  INDEX    DESCRIPTION                       VALUE        MENU
    1)    NUMBER OF CALLS                     300         ANY INTEGER
    2)    TOLERANCE                          0.100E-02    ANY REAL IN (0,1)
    3)    STEP FACTOR                       0.30E+01      ANY REAL > 1
    4)    FAILURES ALLOWED                     4          ANY INTEGER
    5)    PRINTOUT SELECTION                   1          0/1/2
    6)    WALL-PARAMETER                       3          ANY INTEGER
    7)    CANCEL-BUTTON                        1          ( 0/1/2 )
--------------------------------------------------------------------------
     ENTER CHANGES
 ALL VARIABLES FIXED
 ALL VARIABLES FIXED
 ALL VARIABLES FIXED
          NUMBER OF       ROLL   CALLS:          224


     /\/\/\/\/\/\       MERLIN    IS AT YOUR COMMAND !!!
 SHORTDIS
 TOTAL NU. OF CALLS =            225
 NU. OF CALLS SINCE LAST RESET             225
    1) X            .......   3.0000000000000
    2) Y            ....... -0.78958705969091E-38
    3) Z            .......  0.50873126074991E-39
          VALUE.......       0.30930676137554E-73


     /\/\/\/\/\/\       MERLIN    IS AT YOUR COMMAND !!!
 SIMPLEX
--------------------------------------------------------------------------
                              SIMPLEX - PANEL
--------------------------------------------------------------------------
  INDEX    DESCRIPTION                       VALUE        MENU
    1)    INITIALIZATION SCHEME                  1        (1/2)
          (SYSTEMATIC/RANDOM)
    2)    INITIALIZATION TOLERANCE         0.100          ANY REAL
    3)    INIT. CALLS/VARIABLE               100          ANY INTEGER
    4)    SIMPLEX TOLERANCE                0.000E+00      ANY REAL
    5)    SIMPLEX CALLS                      500          ANY INTEGER
    6)    PRINTOUT SELECTION                   1         (0/1/2)
    7)    CANCEL-BUTTON                        1          ( 0/1/2 )
--------------------------------------------------------------------------
     ENTER CHANGES
          NUMBER OF    SIMPLEX  CALLS:         2028


     /\/\/\/\/\/\       MERLIN    IS AT YOUR COMMAND !!!
 SHORTDIS
 TOTAL NU. OF CALLS =            2253
 NU. OF CALLS SINCE LAST RESET             2253
    1) X            .......   3.0000000000000
    2) Y            .......  0.40658440073078-133
    3) Z            .......  0.58722944820820-135
          VALUE.......       0.16838565116755-264
```

```
     /\/\/\/\/\/\      MERLIN    IS AT YOUR COMMAND !!!
 BFGS
--------------------------------------------------------------------------------
                              BFGS - PANEL
--------------------------------------------------------------------------------
  INDEX     DESCRIPTION                        VALUE        MENU
    1)     NUMBER OF CALLS                      300          ANY INTEGER
    2)     TOLERANCE                           0.100E-02     ANY REAL IN (0,1)
    3)     ERROR-BOUND                        0.10E-01       ANY REAL < 1
    4)     USE/RECALCULATE GRADIENT            0             (1/0)
    5)     USE/RESET  HESSIAN                  0             (1/0)
    6)     PRINTOUT SELECTION                  1             0/1/2
    7)     WALL-PARAMETER                      3             ANY INTEGER
    8)     CANCEL-BUTTON                       1             ( 0/1/2 )
--------------------------------------------------------------------------------
     ENTER CHANGES
 ALL VARIABLES FIXED
 ALL VARIABLES FIXED
 ALL VARIABLES FIXED
 ALL VARIABLES FIXED
          NUMBER OF       BFGS  CALLS:          18


     /\/\/\/\/\/\      MERLIN    IS AT YOUR COMMAND !!!
 DFP
--------------------------------------------------------------------------------
                              DFP - PANEL
--------------------------------------------------------------------------------
  INDEX     DESCRIPTION                        VALUE        MENU
    1)     NUMBER OF CALLS                      300          ANY INTEGER
    2)     TOLERANCE                           0.100E-02     ANY REAL IN (0,1)
    3)     ERROR-BOUND                        0.100E-01      ANY REAL IN (0,1)
    4)     USE/RECALCULATE GRADIENT            1             (1/0)
    5)     USE/RESET  HESSIAN                  1             (1/0)
    6)     PRINTOUT SELECTION                  1             0/1/2
    7)     WALL-PARAMETER                      3             ANY INTEGER
    8)     CANCEL-BUTTON                       1             ( 0/1/2 )
--------------------------------------------------------------------------------
     ENTER CHANGES
 ALL VARIABLES FIXED
          NUMBER OF        DFP  CALLS:          0


     /\/\/\/\/\/\      MERLIN    IS AT YOUR COMMAND !!!
 SHORTDIS
 TOTAL NU. OF CALLS =          2271
 NU. OF CALLS SINCE LAST RESET           2271
   1) X           .......   3.0000000000000
   2) Y           .......   0.40658440073078-133
   3) Z           .......   0.58722944820820-135
        VALUE.......        0.16838565116755-264


     /\/\/\/\/\/\      MERLIN    IS AT YOUR COMMAND !!!
 STOP
```