AveTools v3.0 [10-DEC-2014]

ENSDF evaluation tool to calculate averages

T. Kibédi (ANU, e-mail: Tibor.Kibedi@anu.edu.au)

Introduction

The program AveTools combines three different statistical methods to calculate averages of experimental data with uncertainties. These include:

a) LWM - Limitation of Relative Statistical Weight
b) NRM - Normalised Residual Method
c) RT - Rajeval Technique
d) Bootstrap method
e) Mandel-Paule approach

A detailed description of the methods used can be found in the following references:

LWM, NRM, RT	[1992Ra08] M.U. Rajput and T.D. MacMahon, Nucl. Instr. and Meth. in Phys. Res. **A312** (1992) 289
Bootstrap	[2002He06] O. Helene and V.R. Vanin Nucl. Instr. and Meth. in Phys. Res. A481 (2002) 626
Mandel-Paule	[2011Ch22] J. Chen, S.D. Geraedts, C. Quellet, B. Singh Applied Radiation and Isotopes 69 (2011) 1069

The program is based on LWEIGHT v1.3, EV4 and RajNew codes developed by D. MacMahon (Imperial Collage Reactor Centre, London, UK) and E. Browne (LBL, Berkeley, USA). The Mandel-Paule code was developed by J. Chen (McMaster, Canada)

Input data file

The input data is given in blocks. Each block may contain up to 500 data points. A data point contains

a) **Label** (maximum of 40 characters long with NO embedded spaces)
b) **X-value** (a numerical value in free format: 147, 147.0 or 1.47E+2)
c) **Symmetric Uncertainty in Nuclear Data Sheets style** (a maximum of two digits integer)

They can be given in free format separated by space(s) characters, for example:

1969He19 0.00444 21

The structure of a data block is

Title (max 132 characters)
X-title (max 40 character)
1st Data Point
2nd Data Point
….

500th Data Point

Data blocks starting with **# (hash character or number sign)** will be skipped in the numerical calculations. **Lines starting with #** can be used to insert comments into the input file.

The program will verify each data entry. An error message with the line number in the input file will be generated if an error is detected.

In cases, when X-values are identical in a data set, no real calculation can be carried out, however the program will attempt to evaluate the (internal) uncertainties.

Several data blocks cane be combined with a line containing ***NEW** (not case sensitive)

A sample data file (Avetoolst.in) looks like:

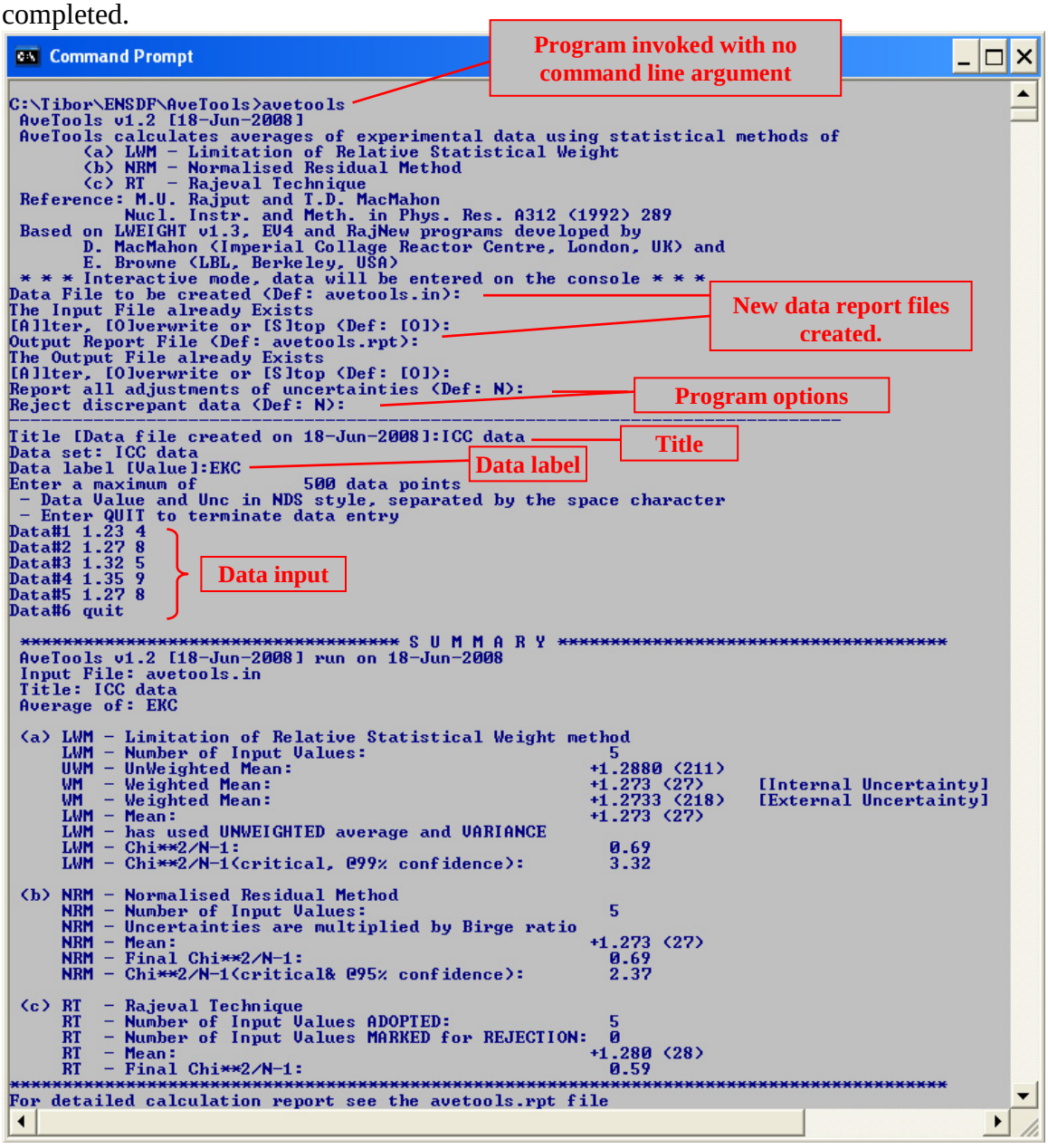
```
198Au T1/2 data from 2011Ch22 J. Chen et al., Appl. Radiat. Isot.
69, 1064 (2011)
T1/2[days]
# User comments can be inserted with a line starting with "#"
# Make sure data entry LABELs have no embedded space character!
# Data points with no uncertainties are excluded
#Amaldi_etal.(1935)                2.7
#McMillan_etal.(1937)              2.7
#Pool_etal.(1937)                  2.5
#Sherr_etal.(1941)                 2.7
Diemer_Groendijk(1946)             2.73     2
#Seren_etal.(1947)                 2.7
#Saxon_(1948)                      2.66     1
Saxon_Heller(1949)                 2.69     2
#Steffan_etal.(1949)               2.7
Cavanagh_etal.(1951)               2.66     1
Sinclair_Holloway(1951)            2.73     1
Silver_(1951)                      2.69     1
Lockett_Thomas(1953)               2.697    3
Bell_Yaffe(1954)                   2.699    3
Tobailem_(1955b)                   2.686    5
#Tobailem_(1955a)                  2.686    5
Johansson_(1956)                   2.697    5
Sastre_Price(1956)                 2.694    6
Keene_(1958)                       2.704    4
Robert_(1960)                      2.699    4
Starodubtsev_etal.(1963)           2.687    5
Anspach_etal.(1965)                2.694    4
Goodier_(1968)                     2.695    7
Lagoutine_etal.(1968)              2.697    5
Reynolds_etal.(1968)               2.693    5
Vuorinen_Kaloinen(1969)            2.695    2
Cabell_Wilkins(1969)               2.6946   10
CostaPaivaandMartinho(1970)        2.696    4
Debertin_(1971)                    2.693    3
Hoppes_etal.(1982)                 2.695    2
Rutledge_etal.(1982)               2.6935   4
Abzouzi_etal.(1990)                2.6966   7
# Unterweger`s 1992 paper superseded
#Unterweger_etal.(1992)            2.69517  21
Mignonsin_(1994)                   2.6837   50
Unterweger_Lindstrom(2004)         2.69573  30
```

```
Lindstrom_etal.(2005)              2.6924   11
Novkovic_etal.(2006)               2.6947   6
Goodwin_etal.(2007)                2.6949   8
Spillane_etal.(2007)               2.706    19
Kumar_etal.(2008)                  2.6971   20
Ruprecht_etal.(2008)               2.6939   4
Fortak_etal.(2010)                 2.684    4
Goodwin_etal.(2010)                2.6948   9
#Lindstrom_etal.(2010)             2.6910   4
# second data set
*NEW
59Co 1099.245 CC
         ECC
 1952ME53 1.94E-4 7
 1953HI02 1.84E-4 27
 1964CO34 1.36E-4 10
```

The minimum number of data points is 2, however the Rajeval Technique is required a minimum of 3 data points.

Terminal dialogue

The program can be run interactively, i.e. no input file is required and the data, including title, label, values and associated uncertainties will be written into the data file. This is shown in the figure below. The user has the choice to use default file names (avetools.in, avetools.rpt) or use different ones. The program options will enable or disable a more detailed list of the calculations and to automatically reject discrepant data. Note, that the data labels are generated automatically, but they can be modified after the program run completed.



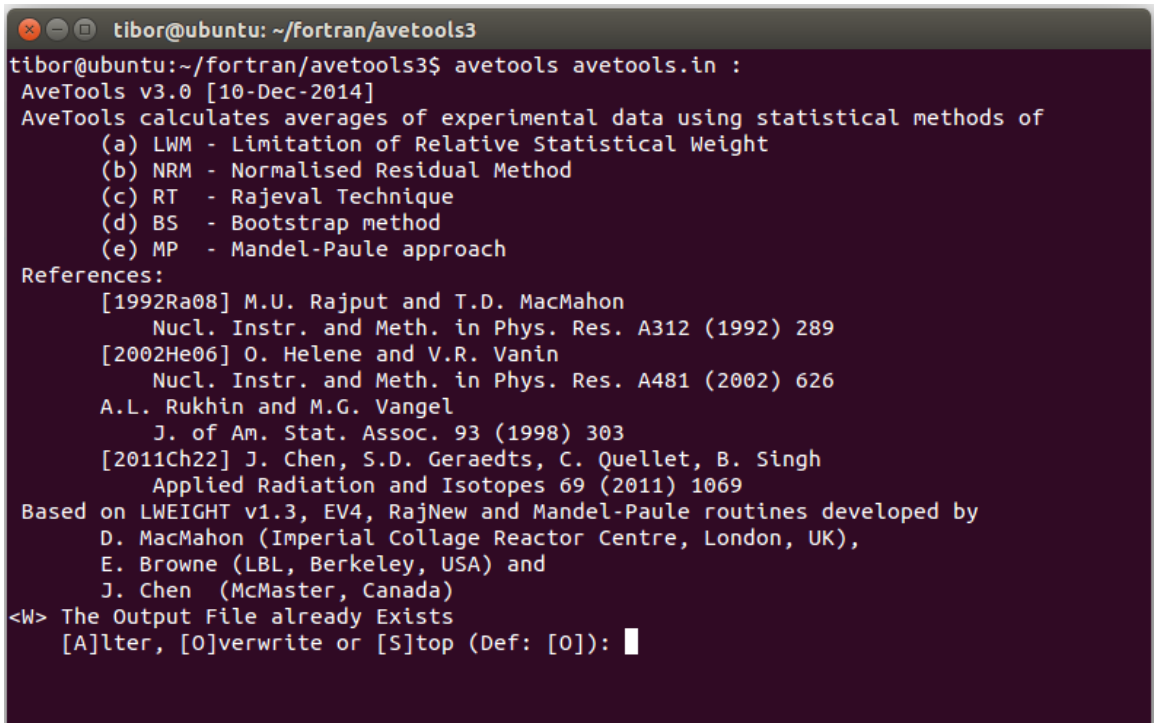
Alternatively all arguments can be given in the command line, including input and output file names, and switches. Using **":"** (colon) instead of the output file name will create an output file name form the input file name by replacing the extension with an "rpt".

Program switches:

- **-a** Report all adjustments of uncertainties
- **-r** Reject (exclude) discrepant data (default: NO)

Typical program dialogue, using the sample input file, Discrepant.in, is shown below (Windows).

Typical program dialogue, using the sample input file, Discrepant.in, is shown below (Linux/Mac OS).



Calculation report file

Detailed calculation report is given for all three statistical methods used, followed by a summary. The calculation summary is displayed on the Terminal console.

Code description

The program is written in FORTRAN. The original numerical procedures of LWEIGHT, EV4 and RAJNEW have been ported to F90 and modified significantly. The program uses a modified version of the NNDClib F90 library (dated November 19, 2003) and kindly provided C.L. Dunford (NNDC).

Critical reduced χ^2 values are evaluated using the DCDFLIB, *"Library of Fortran Routines for Cumulative Distribution Functions, Inverses, and Other Parameters"* (February, 1994) by Barry W. Brown, James Lovato and Kathy Russell, Department of Biomathematics, Box 237, The University of Texas, M.D. Anderson Cancer Center 1515 Holcombe Boulevard Houston, TX 77030.

The program was developed on MS Windows, using MS Visual studio and Intel FORTRAN 90 compiler.

Program distribution and installation

Avetools is distributed for Windows, Linux and MAC OS. The following files are included:

AveTools.exe
AveTools.in (sample input)
AveTools.rpt (calculation report file)
AveTools.pdf (program manual, this file)

Windows all steps of the installation are automated using Inno Setup utility, which will create a program group and append the installation directory to the PATH.

On Linux and MAC the files are distributed as a single TAR file. Please add the installation directory to the path manually.

Please direct all comments and bug reports to Tibor.Kibedi@anu.edu.au