Tutorials and worked examples for simulation, curve fitting, statistical analysis, and plotting.
https://simfit.uk
https://simfit.org.uk
https://simfit.silverfrost.com

1 Options for the number of significant digits in tables

Floating–point numbers (i.e., numbers with a decimal point) are stored by computers in binary form but data files for input into SimFIT and tables output with results are in text format. Given a number x, the range of values allowed by SimFIT for the absolute value of x to 3 significant digits (i.e., 3 digits not counting the decimal point) is

$$2.25 \times 10^{-308} \le |x| \le 1.79 \times 10^{308}$$

and the maximum number of significant digits allowed in this range is approximately 15.

SimFIT will accept data within such limits and performs calculations to double precision but, because all calculations are subject to rounding and truncation errors, only a lower number of significant digits, say 12, is required especially given that most calculations SimFIT performs involve iterative procedures like nonlinear optimisation. Further, scientific instruments are seldom accurate at this level of accuracy and in many cases it is not reasonable to accept results with more significant digits than used to represent the data. Because of the difficulty of reading and writing extremely large numbers there is a format called scientific notation to be explained next.

All floating–point numbers can be written concisely using powers of ten as multiplication factors as follows

$$1000000.0 = 1.0 \times 10^{6}$$
$$0.0000001 = 1.0 \times 10^{-6}$$

where the value and convenience of using powers of ten will be clear at a glance. To avoid superscripts and also to limit the number of characters required to represent numbers, scientific notation simply uses the idea of one digit in front of the decimal point and a fixed number of digits after the decimal point with the code E+ab for $\times 10^{ab}$ and E-ab for $\times 10^{-ab}$. Here for example is the number -1.23456 that unquestionably has 6 significant digits but multiplied by powers of ten as they would be displayed by SimFIT using Option 6 (scientific notation) and Option 7 (standard notation).

Option 6	Option 7
-1.23456E+09	-1.23456E+09
-1.23456E+08	-1.23456E+08
-1.23456E+07	-12345600.0
-1.23456E+06	-1234560.0
-1.23456E+05	-123456.0
-1.23456E+04	-12345.6
-1.23456E+03	-1234.56
-1.23456E+02	-123.456
-1.23456E+01	-12.3456
-1.23456E+00	-1.23456
-1.23456E-01	-0.123456
-1.23456E-02	-0.0123456
-1.23456E-03	-0.00123456
-1.23456E-04	-0.000123456
-1.23456E-05	-0.0000123456
-1.23456E-06	-1.23456E-06
-1.23456E-07	-1.23456E-07

It will be clear that the scientific format has a fixed width with the numbers aligned at the decimal point whereas the numbers in standard notation are of variable width and, when the numbers become rather large or very small, SIMFIT Option 7 resorts to scientific notation.

1.1 The options for results

SIMFIT releases up to version 7 always displayed numbers in scientific notation with a field width and significant digits appropriate for the analysis being employed. To many analysts this is by far the most valuable way to display numbers as the field width is fixed, all numbers are aligned at the decimal points and orders of magnitude can be seen at a glance, but some SIMFIT users find this difficult to understand so from version 8 SIMFIT provides an interface that users can employ to change number format interactively. This is done using the following sequence of steps starting from the [Configure] option from the SIMFIT main page

```
[Configure] --> [Advanced] --> [Change number of significant digits in results tables]
```

which takes immediate effect after choosing the format required without requiring the [Apply] button to be pressed.

The ten options are

```
Option  1:  Up to  12 significant digits
Option  2:  Up to  11 significant digits
Option  3:  Up to  10 significant digits
Option  4:  Up to   9 significant digits
Option  5:  Exactly 7 significant digits
Option  6:  Exactly 6 significant digits (scientific notation)
Option  7:  Exactly 6 significant digits (standard notation: recommended)
Option  8:  Exactly 5 significant digits
Option  9:  Exactly 4 significant digits
Option 10:  Exactly 3 significant digits
```

which all use a field width of 13 characters. For this reason the number of significant digits in options 1 to 4 cannot be exact but are upper limits.

To illustrate the difference between Scientific notation and standard notation consider the results created by SIMFIT after fitting one then two exponentials using SIMFIT program **exfit** to analyse the test file `exfit.tf4` (which has six significant digits) in order to decide if fitting two exponentials after one exponential justifies the higher order model with extra parameters.

1.2 Option 6: Scientific notation

```
 For best-fit 1-exponential function

 Parameter     Value        Std.Error    Lower95%cl    Upper95%cl     p
    A(1)    1.69443E+00  2.67006E-02  1.63974E+00  1.74912E+00  0.0000
    k(1)    1.46094E+00  5.77654E-02  1.34261E+00  1.57926E+00  0.0000
    AUC     1.15982E+00  3.78135E-02  1.08237E+00  1.23728E+00  0.0000
 AUC is the area under the curve from t = 0 to t = infinity
 Initial time point (A)    =  3.59830E-02
 Final time point   (B)    =  1.61100E+00
 Area over range (A,B)     =  9.90210E-01
 Average over range (A,B) =  6.28698E-01
```

```
 For best-fit 2-exponential function

 Parameter     Value       Std.Error    Lower95%cl    Upper95%cl     p
    A(1)    8.52553E-01  6.77105E-02  7.13372E-01  9.91734E-01  0.0000
    A(2)    1.17644E+00  7.47538E-02  1.02278E+00  1.33010E+00  0.0000
    k(1)    6.79334E+00  8.54540E-01  5.03681E+00  8.54987E+00  0.0000
    k(2)    1.11206E+00  5.10959E-02  1.00703E+00  1.21709E+00  0.0000
    AUC     1.18339E+00  1.47096E-02  1.15316E+00  1.21363E+00  0.0000
 AUC is the area under the curve from t = 0 to t = infinity
 Initial time point (A)    =  3.59830E-02
 Final time point   (B)    =  1.61100E+00
 Area over range (A,B)     =  9.38322E-01
 Average over range (A,B) =  5.95754E-01

F test results

WSSQ-previous (WSSQ1)              =  2.24923E+02
WSSQ-current (WSSQ2)               =  2.43970E+01
Number of parameters-previous (M1) =      2
Number of parameters-current (M2)  =      4
Number of data points (NPTS)       =     30
Akaike AIC-previous                =  6.44368E+01
Akaike AIC-current                 =  1.79794E+00
Evidence ratio (ER)                =  3.99818E+13
Schwarz SC-previous                =  6.72392E+01
Schwarz SC-current                 =  7.40273E+00
Mallows Cp                         =  2.13701E+02
Mallows ratio (Cp/M1)              =  1.06851E+02
Numerator degrees of freedom       =      2
Denominator degrees of freedom     =     26
F test statistic (FS)              =  1.06851E+02
p = P(F >= FS)                     =  0.0000
1 - p = P(F =< FS)                 =  1.0000
5% upper tail point                =  3.36902E+00
1% upper tail point                =  5.52633E+00

Conclusion based on F test
Reject previous model at 1% significance level
There is strong support for the extra parameters
Tentatively accept the current best fit model
```

You will observe that all floating point numbers in these results tables have exactly six significant digits and all the numbers are lined up at the decimal point but use exponential notation for powers of ten.

1.3 Option7: Standard notation

Now performing the same analysis after selecting the default Option number 7 leads to the following analysis in which all the floating point numbers are still displaying six significant digits but now in standard format. Note however that, even in standard format, it is necessary to swap to scientific notation when the absolute value of the numbers become very large ($> 10^7$) or very small ($< 10^{-6}$). This is necessary to maintain a maximum width of 13 characters per number in multi–column tables.

For best-fit 1-exponential function

Parameter	Value	Std.Error	Lower95%cl	Upper95%cl	p
A(1)	1.69445	0.0267064	1.63974	1.74915	0.0000
k(1)	1.46101	0.0578035	1.3426	1.57941	0.0000
AUC	1.15978	0.0378344	1.08228	1.23728	0.0000

AUC is the area under the curve from t = 0 to t = infinity
Initial time point (A)   = 0.035983
Final time point   (B)   = 1.611
Area over range (A,B)   = 0.990184
Average over range (A,B) = 0.628681

For best-fit 2-exponential function

Parameter	Value	Std.Error	Lower95%cl	Upper95%cl	p
A(1)	0.852548	0.0677272	0.713332	0.991763	0.0000
A(2)	1.17645	0.0747742	1.02275	1.33015	0.0000
k(1)	6.79344	0.854289	5.03743	8.54946	0.0000
k(2)	1.11206	0.0511103	1.007	1.21712	0.0000
AUC	1.18339	0.0147092	1.15316	1.21363	0.0000

AUC is the area under the curve from t = 0 to t = infinity
Initial time point (A)   = 0.035983
Final time point   (B)   = 1.611
Area over range (A,B)   = 0.938323
Average over range (A,B) = 0.595754

F test results

WSSQ-previous (WSSQ1)   = 224.923
WSSQ-current (WSSQ2)   = 24.397
Number of parameters-previous (M1) = 2
Number of parameters-current (M2) = 4
Number of data points (NPTS)   = 30
Akaike AIC-previous   = 64.4368
Akaike AIC-current   = 1.79794
Evidence ratio (ER)   = 3.99818E+13
Schwarz SC-previous   = 67.2392
Schwarz SC-current   = 7.40273
Mallows Cp   = 213.701
Mallows ratio (Cp/M1)   = 106.851
Numerator degrees of freedom   = 2
Denominator degrees of freedom   = 26
F test statistic (FS)   = 106.851
p = P(F >= FS)   = 0.0000
1 - p = P(F =< FS)   = 1.0000
5% upper tail point   = 3.36902
1% upper tail point   = 5.52633

Conclusion based on F test
Reject previous model at 1% significance level
There is strong support for the extra parameters
Tentatively accept the current best fit model