Tutorials and worked examples for simulation, curve fitting, statistical analysis, and plotting.
http://www.simfit.org.uk

Simulating a data set that is exact to computer precision for a user-defined model is often the first step in simulation, so that random error can be added retrospectively to simulate experimental results.

SimFIT can simulate a very large number of models from user-supplied model files and allows models to include the following procedures.

1. All the standard mathematical operations such powers, logarithms, trigonometric and hyperbolic functions, etc.

2. A very substantial library of special functions including erf, erfc, and Bessel functions, etc.

3. A large number of numerical techniques such as quadrature, root finding, eigenvalues, matrix operations, and convolution of two functions, etc.

4. Systems of differential equations with Jacobians either supplied or approximated numerically.

5. Logical tests for branching.

6. Models that include calls to sub-models.

Such models can also be used for nonlinear regression, and details will be found in the following publication

Using ASCII text files in post-fix notation (reverse Polish) to define mathematical models and systems of differential equations for simulation and nonlinear regression.
Bardsley,W.G. & Prasad,N *Computers and Chemistry* (1997) **21**, 71–82,

but also in the SimFIT reference manual w_manual.pdf, or in user_defined_models.html.

However, it is also possible to use standard mathematical notation in order to define a model as long as the model is contained within a begin{expression} and a end{expression} section as will be demonstrated for the models to be used here. For many of the demonstration model files supplied with SimFIT there are two versions, one in reverse Polish, e.g. usermod1.tf9, and one for the same model but with subscript _e, e.g. usermod1_e.tf9, using standard mathematical expressions.

Choosing the [A/Z] option from the SimFIT main menu is used to open the program **makdat**, which then allows you to create such almost-exact data from a a user-supplied model.

Example 1. Damped simple harmonic motion

For a simple example we will investigate how to simulate damped simple harmonic motion given by

$$f(x) = \exp(-x/2)\cos 5x.$$

For instance, the test file usermod1_e.tf9 has the following model for damped simple harmonic motion

$$f(x) = p_4 \exp(-p_3 x)\cos(p_1 x - p_2)$$

which simply requires choosing the parameters

$$p_1 = 5$$
$$p_2 = 0$$
$$p_3 = 0.5$$
$$p_4 = 1.$$

Model files are simple ASCII text files with a title, details of the number of equations, then the model in reverse Polish, (i.e. last-in first-out which is how computers work and some languages like PostScript), with standard mathematical notation included if required.

Note that the percentage sign(%) is used as a special character to denote change in content, and that there is a SiMFiT program **usermod** to help users develop such models.

The model file and simulated data are shown next.

```
%
Example: user supplied function of 1 variable ... damped SHM
        Damped simple harmonic motion in the form
        f(x) = p(4)*exp[-p(3)*x]*cos[p(1)*x - p(2)]
        where p(i) >= 0
 %
 1 equation
 1 variable
 4 parameters
 %
 begin{expression}
 f(1) = p(4)exp(-p(3)x)cos(p(1)x - p(2))
 end{expression}
 %
```

Damped Simple Harmonic Motion

User-defined model file: USERMOD1.TF9

$y = \exp(-x/2)\cos(5x)$
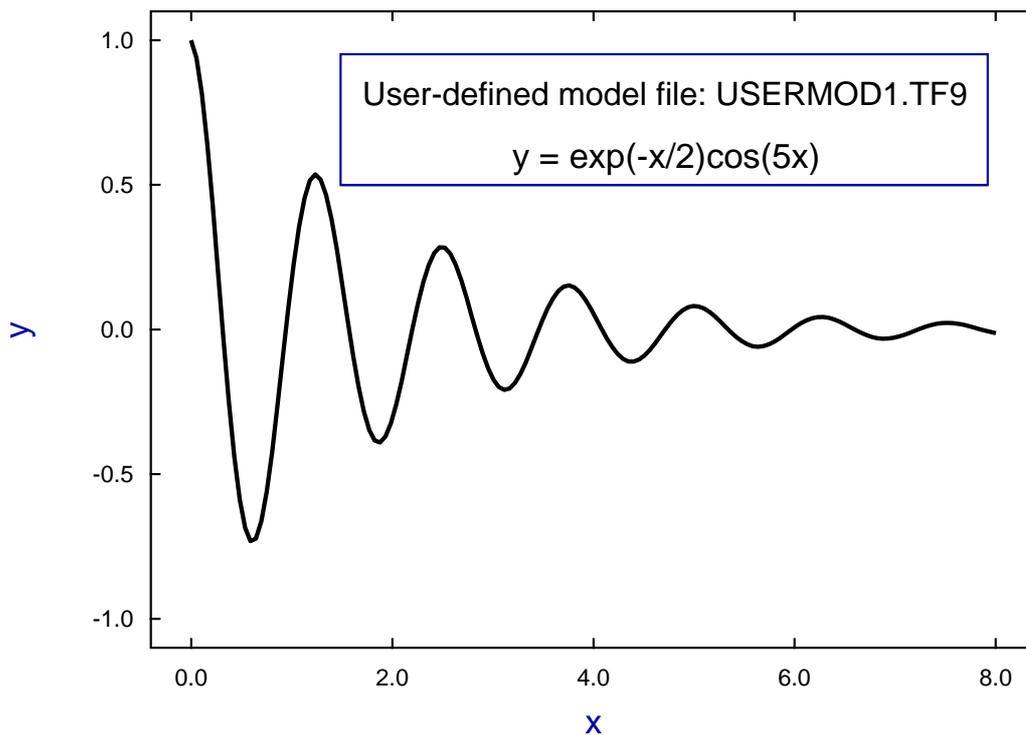
Example 2: Diffusion in a long tube

This example illustrates how to use special functions such as erfc in a user-defined model.

Consider a very long tube of constant cross section filled with solvent but with a barrier separating the tube into two sections with half the tube filled with solute at concentration C_0 as illustrated next, using a coordinate system with the barrier at position $x = 0$.

$$x < 0 \qquad\qquad x = 0 \qquad\qquad x > 0$$
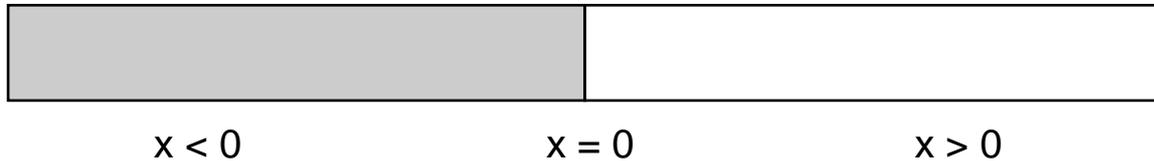
In an idealized situation where the barrier is removed instantaneously at time $t = 0$ with no mixing effect there would be an initial situation as follows

$$C(x, t) = C_0, \text{ for } x < 0$$
$$C(x, t) = \tfrac{1}{2}C_0, \text{ at } x = 0$$
$$C(x, t) = 0, \text{ for } x > 0.$$

If there is no effect operating except for simple diffusion then the concentration subsequently would obey the diffusion equation

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$$

with solution

$$C(x, t) = \tfrac{1}{2}C_0 \operatorname{erfc}\frac{x}{2\sqrt{(Dt)}}.$$

and the SimFIT test file usermod1_e.tf8 shown below contains the text required to simulate this equation.

```
 %
Example: user supplied function of 1 variable ... capillary diffusion

f(x) = p(1)*erfc[x/(2*sqrt(p(2))]

 %
 1 equation
 1 variable
 2 parameters
 %
 begin{expression}
 f(1) = p(1)erfc(x/(2sqrt(p(2))))
 end{expression}
 %
```

With $p_1 = 0.5$ then $p_2 = \sqrt{(Dt)}$ varied the following graph was simulated to illustrate the result of diffusion as a function of distance and time with $p_2 = 0.01, 0.1, 1.0, 10.0, 100.0$, and fixed diffusion constant $D = 1$. Evidently diffusion continues until the concentration everywhere is $\tfrac{1}{2}C_0$.

Diffusion in a Tube: C = (1/2)C$_0$erfc[x/{2√(Dt)}]

Legend:
- √(Dt) = 100.0
- √(Dt) = 10.0
- √(Dt) = 1.0
- √(Dt) = 0.1
- √(Dt) = 0.01
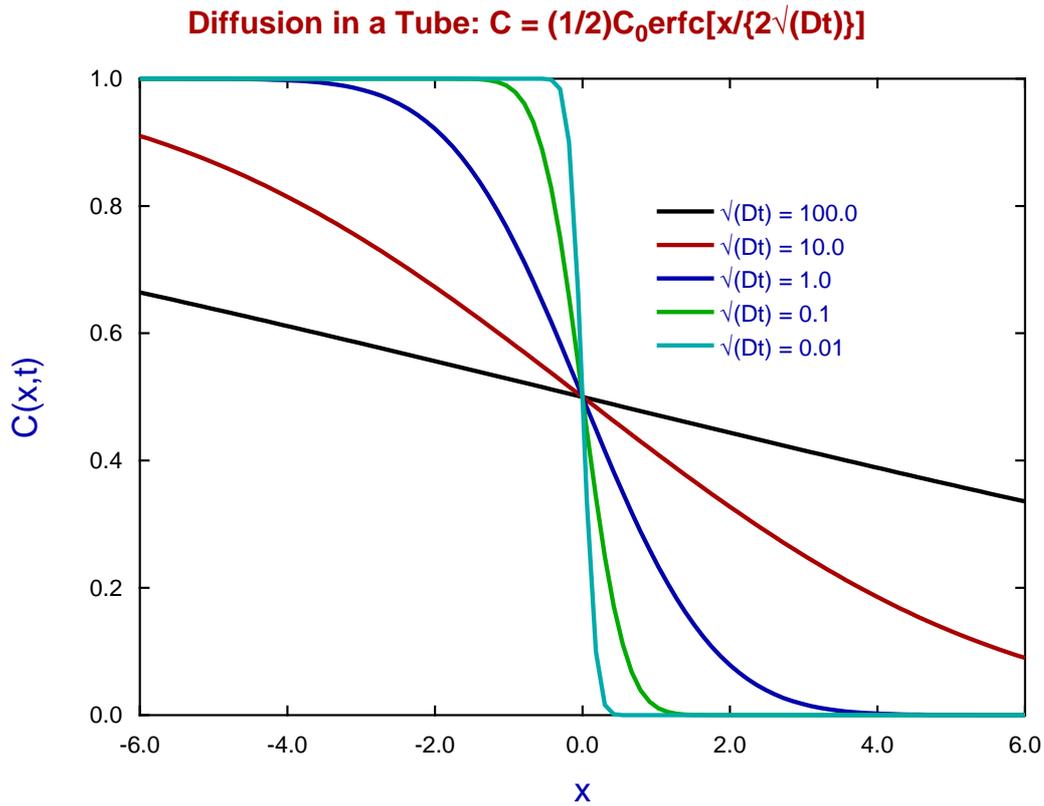
To generate this graph, program **makdat** was used with the range of x fixed at $-6 \leq x \leq 6$, and after each plot the [Advanced] option was used to save each profile as an ASCII text file that was recorded in the graphics project archive. This was then opened by program **simplot** to draw the composite graph above.

Theory

The SIMFIT procedures for user defined models include many one-line commands to evaluate special functions, and the case of the complementary error function used in mode file usermodel_e.tf8 is typical.

Note that the error function erf and the complementary error function erfc are defined as

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-t^2)\, dt$$

$$\text{erf}(-x) = -\text{erf}(x)$$

$$\text{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^\infty \exp(-t^2)\, dt$$

$$\text{erf}(x) + \text{erfc}(x) = 1$$

so that $-1 \leq \text{erf}(x) \leq 1$ and $0 \leq \text{erfc}(x) \leq 2$. As with all special functions listed in the documents w_manual.pdf and user-defined-models.html, these can only be evaluated using numerical techniques.

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