MathCad Functions

**Built-in functions**
- MathCAD has a relatively large number of useful built-in functions
- Trigonometry: $\sin(x), \cos(x), \tan(x), \ldots$
- Truncation and rounding: $\text{floor}(x), \text{ceil}(x), \text{trunc}(x)$
- Log and exponential: $\exp(x), \ln(x), \log(x, [b])$
- File access: $\text{READFILE}, \text{READ_IMAGE}, \ldots$
- Root finding and solving: $\text{root}, \text{polyroot}, \text{lsolve}, \ldots$
- Statistics: $\text{mean}, \text{median}, \text{stdev}, \ldots$
- Regression: $\text{linfit}, \text{expfit}, \text{genfit}, \ldots$
- …

**User-defined functions**
- You can define fairly complex functions in MathCAD using a combination of operators, logical statements, and built-in functions
- Once defined, the functions can be used in your worksheet multiple times

<table>
<thead>
<tr>
<th>Define function</th>
<th>MyFunction (x) := $3x^4 - 2x^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>And use it in a calculation</td>
<td>MyFunction (4) = 736</td>
</tr>
<tr>
<td>And again ...</td>
<td>MyFunction (3) = 225</td>
</tr>
<tr>
<td>And again ...</td>
<td>MyFunction (8) = $1.216 \times 10^4$</td>
</tr>
</tbody>
</table>
Where to Get Built-In Functions

1. From the Calculator Window
   - The simplest functions like square root, inverse, etc.

2. From the "Insert Function" menu
   - Called by "Ctrl-E" or from "Insert" menu
   - Displays a list of functions in different categories

Very useful: Pressing the "?" sign brings up the help window with information about this function.
Calculator Functions

Practice with the calculator functions to produce the following results:

\[
\sqrt{\frac{356 - 24}{13}} = 5.054 \quad \frac{100!}{93! \cdot 7!} = 1.601 \times 10^{10} \quad 3\sqrt{e\pi} = 2.85
\]

\[
3^3 = 7.626 \times 10^{12} \quad \ln(e^{10}) = 10 \quad \log(1024, 2) = 10
\]

\[
\left(1 - \frac{1}{1000}\right)^{1000} = 0.368 \quad \left\lfloor (-18)^3 \right\rfloor = 5.832 \times 10^3
\]
Trigonometry Functions

Remember that:

- The default unit for the angle is **rad** (radian). If you do not specify a unit for the angle, MathCAD will assume it is in radians! Another unit you can use is **deg** (degrees).
- Inverse trigonometric functions will return the angle in radians by default.
  - 90 deg = $\pi/2$ rad (quarter circle)
  - 180 deg = $\pi$ rad (half circle)
  - 360 deg = $2\pi$ rad (full circle)
  - etc.

Example of use

![Diagram of a circle with radians and degrees marked](image)

Convert into radians in your head if you are used to radians:

$$\text{Length}_1 := 7\text{cm} \cdot \sin\left(\frac{\pi}{6}\right)$$

Length $1 = 3.5$ cm

Or use the "deg" unit

$$\text{Length}_2 := 7\text{cm} \cdot \sin(30\text{deg})$$

Length $2 = 3.5$ cm
User-Defined Functions

- Defined similar to a variable but has a list of dummy (undefined) arguments
  \[ \text{Funky}(x, y, z) := \]

- The right side of the equation contains mathematical manipulations on the arguments
  \[ \text{Funky}(x, y, z) := (x + y + z)^2 \]

- Once defined, the function can be used in calculations...
  \[ \text{Funky}(2, 3, 4) = 81 \]

- Or in plots...

Use for XY plots
Rotational Energy Distribution

- **Rotational energy levels of a diatomic**
  - $B$ – rotational constant
  - $I$ – moment of inertia
  - $J_{rot}$ – rotational quantum number ($J = 0,1,2,...$)
  - $R$ – interatomic separation

- **Probability of a given rotational state**
  - $Q$ – rotational partition function
  - $k = 1.38\times10^{-23} \text{J/K}$ – Boltzmann constant

- **Task**
  Assume $B=3.0\times10^{-23} \text{J}$
  Assume $T=300 \text{K}$
  Define and plot the following functions using $J_{rot}$ as a variable:
  - $E(J_{rot})$ – energy of a given rotational quantum state
  - $P(J_{rot})$ – probability to find the molecule in a given rotational quantum state
Solution

\[ T := 300 \text{K} \quad B := 3.0 \cdot 10^{-23} \text{J} \quad k := 1.38 \cdot 10^{-23} \frac{\text{J}}{\text{K}} \]

\[ E(J_{\text{rot}}) := B \cdot J_{\text{rot}} \cdot (J_{\text{rot}} + 1) \]

\[ P(J_{\text{rot}}) := \frac{2 \cdot J_{\text{rot}} + 1}{k \cdot T} \exp \left[ \frac{-B}{k \cdot T} \cdot J_{\text{rot}} \cdot (J_{\text{rot}} + 1) \right] \]

**Things to watch out for:** (1) MathCad selects the ranges for variables in plots automatically. Oftentimes, the MathCAD's choice is not what you want. In such cases, you have to reset the scale manually. (2) Most MathCAD functions do not accept arguments with units. If you want to avoid problems it may be safer to do your calculation without using units explicitly.
Plotting Multiple Functions

- Multiple functions can appear in the same graph. Simply separate them with commas when entering them in the Y-axis placeholder.
- Practice: define and plot functions corresponding to radial wavefunctions of hydrogen atom for $\rho = 0$-20:

$$H - \text{atom wavefunctions ( } \rho=2Zr/a0)$$

$$\Psi_{1s}(\rho) := 2\exp\left(-\frac{\rho}{2}\right)$$

$$\Psi_{2s}(\rho) := \frac{1}{2\sqrt{2}}\left(2 - \frac{\rho}{2}\right)\exp\left(-\frac{\rho}{4}\right)$$

$$\Psi_{3s}(\rho) := \frac{1}{9\sqrt{3}}\left(6 - 2\rho + \frac{\rho^2}{9}\right)\exp\left(-\frac{\rho}{6}\right)$$
Conditional Statements

Sometimes, it is necessary to assign a different value to a function depending on the value of a previous calculation. **IF** function is used for this purpose.

\[
\text{if(condition, truevalue, falsevalue)}
\]

- Practice: define a function that is:
  \[
  = x \text{ for } |x|<1 \\
  = 1 \text{ for } x\geq 1 \\
  = -1 \text{ for } x\leq-1
  \]
- Plot both functions to make sure they do what you expect. Select appropriate x,y-scales to make the functions clearly visible.

\[
F_2(x) := \text{if}( |x| < 1, 1, 0) \\
F_1(x) := \text{if}( |x| < 1, x, \text{sign}(x))
\]

Additional practice: define and plot a function that is:
\[
=x^2 \text{ for } |x|<1 \\
=1 \text{ for } x\geq 1
\]
Random Numbers

Random numbers are required in many calculations, e.g., Monte-Carlo simulations of molecular motion. MathCAD provides several useful random number generators. We will practice with the simplest one:

Function \textit{rnd}(x) produces uniformly distributed random number between 0 and \(x\)

- Define the function \textit{Uniform}(\textit{dummy}) := \textit{rnd}(1)
- Plot it over the \textit{dummy} variable range of -1 to 1
- The result is so called "white noise"
Plotting Two-Dimensional Functions

Functions of two variables can be plotted in three dimensions.

• Define the function $\text{Test}(x,y):=x^2-y^2$ (function that looks like a "saddle")
• Generate a surface plot of Test over the x and y range of -6 to 6
• Set rotation to 0, tilt to 30, and twist to 30
• Rotate it manually to view the plot from all angles
• Now generate a contour plot of Test with a color map

$\text{Test}(x, y) := x^2 - y^2$
Practice: 3D plotting

- Define/plot function:
  \[ \Psi(x, y) = \frac{1}{\sqrt{\pi}} e^{-\frac{x^2+y^2}{2}} \]

- Define function and generate its contour and surface plots:
  \[ \Omega(x, y) = \sin(\sqrt{x^2+y^2}) \]