THE ROLE OF SMARTPHONES AND TABLETS IN NUMERICAL PROBLEM SOLVING

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Introduction

Numerical problem solving was introduced into the Chemical Engineering education and practice in the early nineteen sixties (Shacham et al. 1996). At that time, Fortran or other source code programming languages were used to implement the numerical solution algorithms on "mainframe" computers. Starting in the mid 1980's, the emphasis shifted to the use of general purpose mathematical software packages, such as MAPLE, MATHCAD, MATLAB, Mathematica and PolyMath for numerical problem solving using the PCs and MACs. Mathematical software packages are currently used for routine numerical problem solving in engineering education and practice (Cutlip et al., 1998, Shacham and Cutlip, 1999) as they are easy to use and provide the most time efficient route for obtaining accurate solutions.

The dominant position of the PC and MAC in the personal computing field has been challenged lately by the mobile devices such as smartphones and tablets. Furthermore, it is predicted that by 2017 the dominant operating system for all computing devices will be Google's Android (Wingfield, 2013). Relying on these trends and predictions, we decided to check the possibility of the use of Android-based smartphones, tablets and computers for general numerical problem solving. For this aim, we have developed the PolyMathLite (PML) application for Android-based devices. This app is a slightly simplified version of the Polymath software package (PolyMath is a product of Polymath Software http://www.polymath-software.com). It is significant that the numerical algorithms used in PML are essentially the same and provide the same efficient and accurate solutions as those employed in PolyMath for the PC.
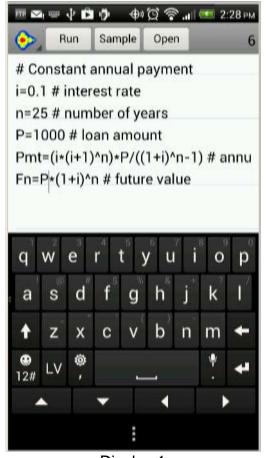
PolyMathLite enables users to obtain numerical solutions to a wide range of problems from relatively simple ones that may be appropriate for users taking advanced level coursework in high school to much more complex courses found in technical schools, colleges, and universities. It will be very applicable for the STEM areas of study namely science, technology, engineering and mathematics. It can even support academic programs and research at the MSc or PhD levels. PML eliminates the dependence on computers and the internet for solving problems numerically, thus solutions can be worked out in regular classrooms as part of a recitation session or an exam. Travel and waiting time can be efficiently utilized for problem solving. No internet connection is required for setting up or achieving problem solutions. The solution is obtained using the most sophisticated solution algorithms and the results are presented in tabular and graphical forms for easy interpretation. When satisfactory versions of the problem definition and its solutions are reached, they can be saved on the Android smartphone, tablet or computer. They can also be shared with external applications such as e-mail, text viewers, cloud storage devices, etc. and integrated into reports and presentations.

In the following examples, the use of PLM for setting up and solving several general types of numerical problems will be demonstrated for two extremes - a very simple and a fairly complex example.

Create your own sophisticated calculator

There are calculations involving one or several explicit algebraic equations which must be carried out frequently for different parameter values. PML enables setting up the system of equations, solving it for one set of parameter values and saving it for future use. The problem can be reloaded, whenever necessary, and resolved for different sets of parameter values.
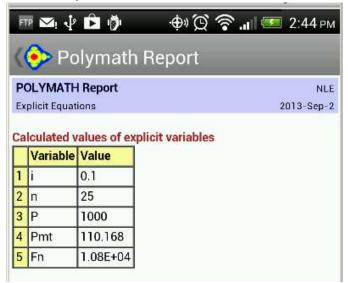
Consider for example a problem involving the calculation of constant annual payment (*Pmt*) and future value (*Fn*) for a loan with amount of *P*, to be repaid in *n* years with interest rate of *i*. The parameters of this problem are: *P*, *n* and *i*. Setting $P = 1000$, $n = 25$ and $i = 10\%$ the problem can be entered into PML as shown in phone Display 1 along with the on-display entry keyboard.

Display 1

Note that the # sign indicates a user comment section. The text in the first line must contain a comment which is used for the problem identification and reload when a problem is saved. Except in the first line, PML disregards the text inserted after the # sign. The constant definitions and the explicit equations can be entered in any order as PML reorders the equations according to the computational sequence. The problem is solved by a tap on the

"Run" button. If there are errors in the problem code syntax, then feedback is given along with the line numbers. When the problem is entered correctly, the PML report that contains the variable values at the solution is presented as shown in Display 2. In this particular case the solution is: *Pmt* = $110 and *Fn* = $10800.

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‹⊙› Polymath Report

| POLYMATH Report | NLE |
| Explicit Equations | 2013-Sep-2 |

Calculated values of explicit variables

	Variable	Value
1	i	0.1
2	n	25
3	P	1000
4	Pmt	110.168
5	Fn	1.08E+04

Display 2

The problem can be saved with the title of "# Constant annual payment" and rerun with different parameter values whenever necessary.

A more complex problem consisting of explicit (only) equations involves, for example, the preparation of a calculator for temperature dependent liquid properties of the water between the melting point and the critical temperature. The following set of equations can carry out those calculations.

```
# Physical property calculator for water (liquid)
# Valid Temperature Range: 273.16K to 647.096K
HVP_H2O = 52053000 * (1 - T / 647.096) ^ (0.3199 - 0.212 * T / 647.096 + 0.25795 * (T / 647.096) ^ 2)
# J/kmol (Uncertainty < 1%)
LDN_H2O = 17.863 + 58.606 * (1 - T / 647.096) ^ 0.35 - 95.396 * (1 - T / 647.096) ^ (2/3)+ 213.89 * (1 -
T / 647.096) - 141.26 * (1 - T / 647.096) ^ (4/3) # kmol/m^3 (Uncertainty < 1 %)
VP_H2O = exp(73.649 - 7258.2 / T - 7.3037 * ln(T) + 4.1653E-06 * T ^ 2) # Pa (Uncertainty < 0.2%)
# Valid Temperature Range: 273.16K to 533.15K
LCP_H2O = 276370 - 2090.1 * T + 8.125 * T ^ 2 - 0.014116 * T ^ 3 + 9.3701E-06 * T ^ 4 # J/kmol*K
(Uncertainty < 1%)
# Valid Temperature Range: 273.16K to 633.15K
LTC_H2O = -0.432 + 0.0057255 * T - 8.078E-06 * T ^ 2 + 1.861E-09 * T ^ 3 # W/m*K (Uncertainty < 1%)
# Valid Temperature Range: 273.16K to 646.15K
LVS_H2O = exp(-52.843 + 3703.6 / T + 5.866 * ln(T) - 5.879E-29 * T ^ 10) # Pa*s (Uncertainty < 3%)
T=300 #K
```
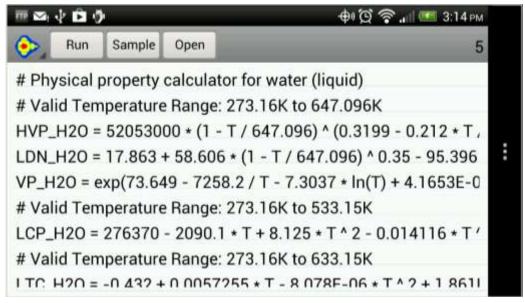
Table 1

This set of equations is so large that the display needs to be adjusted with the use of the finger to locate the portion of the equation set that is of interest. The display showing the upper left of the equation set is shown in Display 3.

Display 3

This use of PLM as a "calculator" provides the following property values: heat of vaporization (HVP_H2O), liquid density (LDN_H2O), vapor pressure (VP_H2O), heat capacity (LCP_H2O), thermal conductivity (LTC_H2O) and viscosity (LVS_H2O). The source of the equations representing the various properties is the DIPPR database (Rowley et al., 2010). DIPPR provides, also, uncertainty estimates on the calculated values and temperature range of validity for the equations. For most properties the temperature range is from the melting point (273.16 K) to the critical point (647.096 K). For some of the properties (LCP_H2O, LTC_H2O and LVS_H2O), the upper limit is slightly lower than the critical temperature. Selecting a temperature value (T = 300 K, in this case) and tapping the "Run" button yields the results given in Display 4. Note that the temperature-dependent equations like those of Table 1 would be very useful in problems where the temperature is changing during the calculations.

POLYMATH Report
Explicit Equations

Calculated values of explicit variables

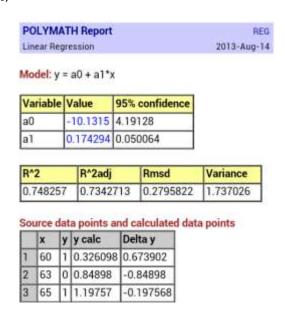|	Variable	Value
1	T	300
2	HVP_H2O	4.38E+07
3	LDN_H2O	55.1762
4	VP_H2O	3537.45
5	LCP_H2O	7.54E+04
6	LTC_H2O	0.608877
7	LVS_H2O	0.000876

Fitting Lines, Curves, and Equations to Data

Computations involving the fitting of a straight line, a polynomial or a complex mathematical model to data (regression) are very widely used in many disciplines. The textbook of Montgomery and Runger (2011) contains examples involving regressions from the disciplines of biology, chemistry, physics, economics, medicine, sports and chemical, civil, mechanical, electrical, industrial, materials, energy and environmental engineering.

Linear Regression - A medical related example presented by Montgomery and Runger (2011) involves, for example, the fitting of a linear regression model to the relationship between hypertension (blood pressure rise in mm of mercury, **y**) and the noise level (in decibels, **x**). The problem can be specified in PML as shown below in Display 5.
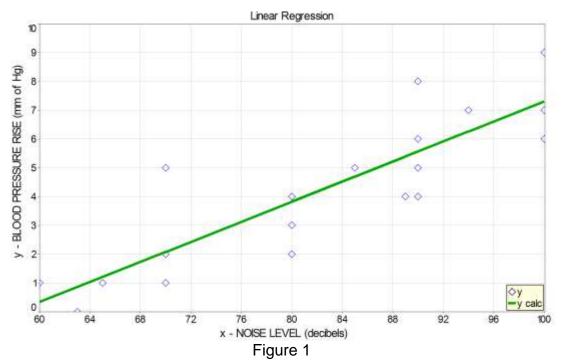
Run	Sample	Open		4

```
# Relationship between noise exposure (x)
# and hypertension (y)
#   y = a0 + a1*x
# Verified solution a0 = -10.1315, a1 = 0.174294
x = [60, 63, 65, 70, 70, 70, 80, 90, 80, 80, 85, 89, 90, 90, 90, 90, 94
y = [1, 0, 1, 2, 5, 1, 4, 6, 2, 3, 5, 4, 6, 8, 4, 5, 7, 9, 7, 6]
polyfit x, y, 1
```

Display 5

The **x** and **y** data are entered in an array format (only part of the **x** data are shown). The command "polyfit x, y, 1" specifies that a 1st degree polynomial (straight line) is sought. The solution report for the problem (see below) displays the numerical values of the model parameters a_0 and a_1, the statistical measures for the goodness of the fit: the correlation coefficient (R^2), the confidence intervals and the variance). The solution report includes, also, a table containing the observed (measured) **y** values, the predicted **y** values (y_{calc}) and the residuals (Delta y = y - $\underline{y}_{calc}$).

POLYMATH Report   REG
Linear Regression   2013-Aug-14

Model: y = a0 + a1*x

Variable	Value	95% confidence
a0	-10.1315	4.19128
a1	0.174294	0.050064

R^2	R^2adj	Rmsd	Variance
0.748257	0.7342713	0.2795822	1.737026

Source data points and calculated data points

	x	y	y calc	Delta y
1	60	1	0.326098	0.673902
2	63	0	0.84898	-0.84898
3	65	1	1.19757	-0.197568

Display 6

A quick analysis of the adequacy of the linear model to represent the data can be obtained by visual inspection of the plot of y and y_{calc} versus x in Figure 1. The data for such a plot containing the values of the dependent and independent variables can be exported to plotting utilities. We have been using of the Plotim application for this purpose. Plotim Free Graphs and Plotim Graph Maker are Android applications available from Google Play.

Figure 1

This plot demonstrates, indeed, that the blood pressure rise increases linearly with the increase of the noise level.

Nonlinear Regression - The regression package of PLM can carry out linear, multiple linear, polynomial and nonlinear regressions. In the following example nonlinear regression is used to calculate the values of the reaction rate coefficient: k_s and the equilibrium constant K_{CH4} for a catalytic reaction where data of the reaction rate (r, in g-mol/hr·gm*10^3) vs. the partial pressures of the reactants and products (P_{CH4}, P_{H2o}, P_{CO2} and P_{H2}, in atm) are available.

```
# Catalytic Reforming Reaction
# Verified Final Values:  ks = 0.002784, KCH4 = 101.999
# Ref.:Prob. 3.10 in  Cutlip and Shacham (2008)
PCH4 = [0.06298, 0.03748, 0.05178, 0.04978, 0.04809, 0.03849, 0.03886, 0.0523, 0.05185, 0.06432, 0.09609]
PH2O = [0.23818, 0.26315, 0.29557, 0.23239, 0.29491, 0.24171, 0.26048, 0.26286, 0.33529, 0.24787, 0.28457]
PCO2 = [0.0042, 0.00467, 0.00542, 0.00177, 0.00655, 0.00184, 0.00381, 0.05719, 0.00718, 0.00509, 0.00652]
PH2 = [0.01669, 0.01686, 0.02079, 0.07865, 0.02464, 0.06873, 0.0148, 0.01635, 0.0282, 0.02055, 0.02627]
r = [0.00013717, 0.00015584, 0.00020028, 5.7E-05, 0.0002015, 7.887E-05, 0.00014983, 0.00015988,
0.00026194, 0.00014426, 0.00020195]
nlinfit r = ks*KCH4*(PCH4*PH2O^2-PCO2*PH2^4/5.051e-5)/(1+KCH4*PCH4)
m(ks)=1
m(KCH4)=1
```
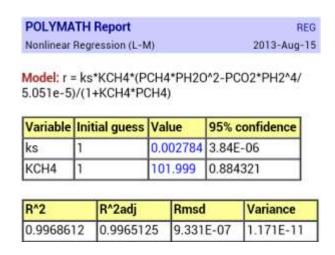
Table 2

The Levenberg-Marquardt algorithm (see, for example, Seber and Wild, 2003) is used to find the optimal parameter values. The PML report (see below) shows correlation coefficient of R^2 = 0.997 and confidence intervals which are much smaller in absolute values than the corresponding parameter values. These results indicate that that the nonlinear model and the calculated parameter values represent well the experimental data.

POLYMATH Report REG

Nonlinear Regression (L-M) 2013-Aug-15

Model: r = ks*KCH4*(PCH4*PH2O^2-PCO2*PH2^4/ 5.051e-5)/(1+KCH4*PCH4)

Variable	Initial guess	Value	95% confidence
ks	1	0.002784	3.84E-06
KCH4	1	101.999	0.884321

R^2	R^2adj	Rmsd	Variance
0.9968612	0.9965125	9.331E-07	1.171E-11

Display 7

Modeling Dynamic Behavior

Differential equations (in particular ordinary differential equations, ODE's) are used for modeling dynamics of processes. One such model, frequently used in ecological studies, is the predator-prey model. The model determines the population over time of the two different species given parameters relating to the interaction between them. Consider for example the version presented in the website: http://demonstrations.wolfram.com/PredatorPreyModel/.

In this example the predators are foxes (with population: *F*) and the preys are rabbits (with population: *R*). Rabbits, which live on vegetation, grow at a rate proportional to the current population: *aR* and die from encounters with Foxes given by *-αRF.* Foxes grow at a rate proportional to the encounters with rabbits, *βRF*, and die at a rate proportional to the current population, *-cF.* The problem definition as entered into PML (including the parameter values and initial and final values of the variables) is the following.

```
# Predator-Prey Model
d(R)/d(t)=a*R-alpha*R*F # Balance on Rabbit Population
R(0)=1 # Initial Condition of Rabbit Population
d(F)/d(t)=beta*R*F-b*F # Balance on Fox Population
F(0)=0.5 # Initial Condition of Fox Population
#Current Parameter Values :
a=1
alpha=0.5
b=0.75
beta=0.25
t(0)=0 # Initial Condition for Independent Variable
t(f)=15 # Final Value for Independent Variable
```
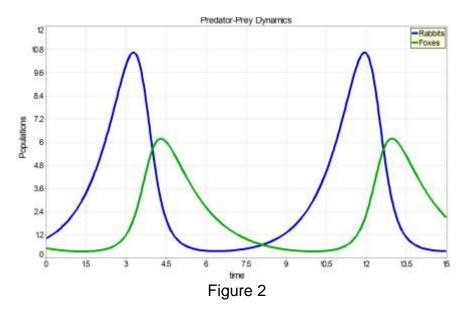
Table 3

The solution obtained is presented in Figure 2 that displays the variation of the rabbit and fox population vs. time. Observe that the population profiles of the rabbits (R) and the foxes (F) at the solution are cyclic and out of phase with each other.
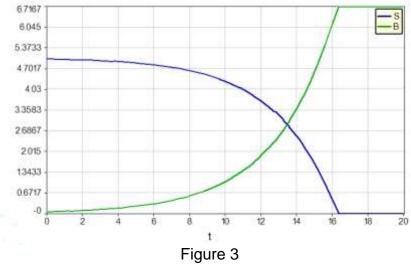

Figure 2

More challenging ODE related problems can be solved by PML, including stiff systems of ODEs, differential-algebraic systems of equations, partial differential equations (using the method of lines) and two point boundary value problems.

Consider for example a batch process of growth of biomass (*B*) from substrate (*S*), presented by Cutlip and Shacham (2008). The model equations, the parameter values and the initial and final values of the variables are shown in the Polymath report shown in Display 8. For this problem one of the eigenvalues of the matrix of partial derivatives becomes very large ($< 1.5*10^6$) in absolute value for t > 16 requiring the use of a special stiff integration algorithm that is available in both PolyMath and PolyMathLite.

POLYMATH Report   DEQ

Ordinary Differential Equations   2013-Aug-15

Calculated values of DEQ variables

	Variable	Initial value	Final value	Minimal value	Maximal value
1	B	0.05	6.71667	0.05	6.71667
2	k	0.3	0.3	0.3	0.3
3	Km	1.0E-06	1.0E-06	1.0E-06	1.0E-06
4	S	5	-1.17E-32	-1.67E-25	5
5	t	0	20	0	20
6	y	0.75	0.75	0.75	0.75

Differential equations

1 $d(S)/d(t) = -k * y * B * S / (Km + S)$

2 $d(B)/d(t) = k * B * S / (Km + S)$

Display 8

The plots of the substrate and biomass amounts versus time, as obtained by PLM, are shown in Figure 3. Observe that slightly above t = 16 the substrate amount reaches zero value and starting this point both the substrate and biomass amounts remain constant. Keeping these values constant requires a properly tuned local truncation error control algorithm; otherwise, the substrate amount will obtain increasing negative values and the biomass amount may grow indefinitely.

Figure 3

Solve Complex Problems

Solution of systems of nonlinear algebraic equations (NLE) is considered a very challenging problem. PML provides several advanced tools for solving systems of NLEs. A simple example that requires solution of a system of NLEs is depicted in Figure 4.
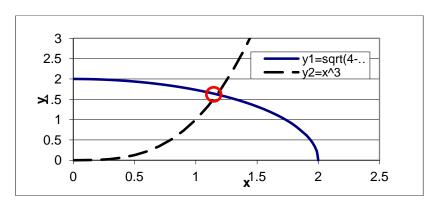

Figure 4 - Finding the intersection point of two curves.

This problem involves finding the intersection of the two curves $y_1 = \text{sqrt}(4-x^2)$ and $y_2 = x^3$ within the first quadrant. Noting that at the intersection $y_1 = y_2 \equiv y$ the equations can be rewritten in implicit forms: $f_1(x,y) = x^2 + y^2 - 4 = 0$ and $f_2(x,y) = y - x^3 = 0$. The solution satisfying these equations can be easily calculated by PLM. Initial estimates for the values x and y should be provided in the first quadrant, and the solution is found in the "Polymath Report" shown in Display 9. The results presented include the values of x and y at the intersection point, and the values $f_1(x,y)$ and $f_2(x,y)$ are very close to zero at the solution.

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POLYMATH Report

Nonlinear Equations   2013-

Calculated values of NLE variables

	Variable	Value	f(x)	Initial Guess
1	x	1.17422	4.7E-10	1
2	y	1.61901	-1.6E-09	1

Nonlinear equations

1 $f(x) = x^2 + y^2 - 4 = 0$

2 $f(y) = y - x^3 = 0$

Display 9

```
# Complex Chemical Equilibrium
R = 1.9872
sum = H2 + O2 + H2O + CO + CO2 + CH4 + C2H6 + C2H4 + C2H2
f(lamda1) = 2 * CO2 + CO + 2 * O2 + H2O – 4 # Oxygen balance
f(lamda2) = 4 * CH4 + 4 * C2H4 + 2 * C2H2 + 2 * H2 + 2 * H2O + 6 * C2H6 – 14 # Hydrogen
balance
f(lamda3) = CH4 + 2 * C2H4 + 2 * C2H2 + CO2 + CO + 2 * C2H6 – 2 # Carbon balance
f(H2) = ln(H2 / sum) + 2 * lamda2
f(H2O) = -46.03 / R + ln(H2O / sum) + lamda1 + 2 * lamda2
f(CO) = -47.942 / R + ln(CO / sum) + lamda1 + lamda3
f(CO2) = -94.61 / R + ln(CO2 / sum) + 2 * lamda1 + lamda3
f(CH4) = 4.61 / R + ln(CH4 / sum) + 4 * lamda2 + lamda3
f(C2H6) = 26.13 / R + ln(C2H6 / sum) + 6 * lamda2 + 2 * lamda3
f(C2H4) = 28.249 / R + ln(C2H4 / sum) + 4 * lamda2 + 2 * lamda3
f(C2H2) = C2H2 – exp(-(40.604 / R + 2 * lamda2 + 2 * lamda3)) * sum
f(O2) = O2 – exp(-2 * lamda1) * sum
H2(0) = 5.992
O2(0) = 0.0001 > 0
H2O(0) = 1
CO(0) = 1
CH4(0) = 0.001 > 0
C2H4(0) = 0.001 > 0
C2H2(0) = 0.001 > 0
CO2(0) = 0.993
C2H6(0) = 0.001 > 0
lamda1(0) = 10
lamda2(0) = 10
lamda3(0) = 10
```

Table 4

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The NLE solver program of PML is able to solve extremely complex and challenging problems belonging to NLE system category. Consider for example the "Complex Chemical Equilibrium" (Problem 4.5 in Cutlip and Shacham, 2008) where the system of equations is shown in Table 4. In this system there are twelve implicit equations with the same number of unknowns.

A major challenge in this problem is that some of the variables are constrained to strictly positive values as their logarithm (which is undefined for values ≤ 0) needs to be calculated. One of the NLE solver algorithms available in PML (the constrained algorithm of Shacham, 1984) is specifically aimed toward solving this kind of "constrained" systems of NLEs. The PML report in Display 10 shows that very accurate solution has been obtained where concentrations of some of the variables in the nonlinear equations (O_2, C_2H_2, C_2H_4 and C_2H_6) are indeed very close to zero.

POLYMATH Report

Nonlinear Equations   2013-Au

Calculated values of NLE variables

	Variable	Value	f(x)	Initial Guess
1	C2H2	3.16E-10	2.6E-25	0.001
2	C2H4	9.54E-08	-2.6E-13	0.001
3	C2H6	1.67E-07	-1.7E-13	0.001
4	CH4	0.066564	-6.7E-16	0.001
5	CO	1.38852	-1.6E-15	1
6	CO2	0.544918	5.6E-15	0.993
7	H2	5.34523	0.0E00	5.992
8	H2O	1.52165	-1.8E-15	1
9	lamda1	24.4197	0.0E00	10
10	lamda2	0.253059	0.0E00	10
11	lamda3	1.55983	0.0E00	10
12	O2	5.46E-21	-4.9E-27	0.0001

	Variable	Value	Initial Value
1	R	1.9872	1.9872
2	sum	8.86687	8.9891

Display 10

Conclusions

An application for numerical solution of problems (PolyMathLite, PML), for Android-based smartphones, tablets and computers, has been developed. This paper has demonstrated that this app is able to efficiently utilize numerical methods to:

- solve problems represented by sets of explicit linear and nonlinear equations
- solve systems of nonlinear algebraic equations (which may also include constraints on selected variables)
- identify the parameter values and calculate statistical metrics for linear, multiple linear, polynomial, and general nonlinear regression problems

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- solve stiff and non-stiff systems of ordinary differential equations
- provide solution results in numerical, tabular and graphical formats that allow for clear presentation and rapid interpretation

The PolyMathLite application has been applied to problems of various complexity levels. Use of the software can be introduced starting with problems that may be appropriate for users with only high school education background at the AP levels in the sciences, math and introduction to engineering. More complex problems can be easily solved by students in the STEM subject areas (science, technology, engineering, and mathematics) in technical programs, community colleges, and four-year colleges and universities. Available PolyMath PC software that builds upon PML enables the solutions to very complex problems found in advanced coursework and in graduate scientific and engineering studies at the MS or PhD levels. Practicing engineers and scientists can use the PolyMath professional software for complex problem solving.

The availability of the PML app on smartphones, tablets and computers introduces users to numerical problem solving that is widely used in the real world. Interest in the application of mathematics should be enhanced and this hopefully may be encouraging to students to enter the STEM fields of study. Problem solving on readily-available hand-held devices will reduce the need to be tied to a computer for solving problems involving numerical computation. There are many future educational possibilities and workplace utilizations of the capabilities that will be enabled by this type of calculational tool that can be as close as a smartphone.

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