

GC 2008-266: EFFECTIVE AND LOW-COST NUMERICAL PROBLEM SOLVING SOFTWARE FOR ENGINEERING EDUCATION

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EFFECTIVE AND LOW-COST NUMERICAL PROBLEM SOLVING SOFTWARE FOR ENGINEERING EDUCATION

Engineering education increasingly involves problem solving that requires numerical solutions of complicated systems of equations and/or regressions/curve fitting of extensive data. Software required for these types of problems can be expensive for academic departments, and typically it can be very expensive for individual graduates when they start their professional careers.

Many developing engineering programs have limited resources to provide this type of software for their faculty and students, and the latest personal computers that enable this software problem solving are in limited supply.

A possible solution to this challenge in the advancement of global engineering education is to be enabled by philanthropic cooperation of the non-profit educational corporation with the name of Computer Aids for Chemical Engineering Education (the CACHE Corporation¹) and Polymath Software². These two organizations have been providing low-cost site licenses of POLYMATH to mainly chemical engineering departments since 1990, with currently some 110 site licenses in use by universities world wide with most institutions being located in the USA.

A new initiative that provides these site licenses, at special low or no cost to interested engineering departments or programs in developing countries is presented in this paper. This initiative will enable interaction numerical problem solving on a wide range of personal computers. These site licenses will allow distribution of individual copies of the software to all students, faculty and staff. In addition, the software may be installed in engineering computer labs and laboratories.

POLYMATH Software – A Brief Overview

POLYMATH enables the user to apply effective numerical analysis techniques during interactive problem solving on personal computers with Microsoft³ operating systems from Windows 95³ through Vista³. This software is extremely easy to use as there is no command language to remember. Results are presented in tabular or graphical formats for easy understanding and for incorporation into papers and reports. Capabilities now include a color-coded full-screen editor and allow for solution of problems involving Linear Equations, Nonlinear Equations, Differential Equations, Data Analysis and various types of Regression. Capabilities of POLYMATH are summarized in Table 1. The installation file is relative small, about 17 Mb, and the installed code requires only 9 Mb.

POLYMATH Software – A Very Simple Example

Let's consider a simple example of a model of a well-mixed batch reactor that is described by a system of ordinary differential equations. The batch reactor initially has only reactant A. The reactions are first order and irreversible. This example will be solved with all three software packages.

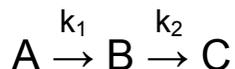


Table 1 – POLYMATH Educational Version

- Linear Equations - up to 100 simultaneous equations.
- Nonlinear Equations - up to 30 simultaneous nonlinear and 40 explicit algebraic equations
- Differential Equations - up to 30 simultaneous ordinary differential and 40 explicit algebraic equations
- Data analysis and Regression - up to 300 data points with capabilities for linear, multiple linear, and nonlinear regressions
- Automatic Creation of Excel Spreadsheet Solution for Problem (include unique ODE_Solver Add-In for solving simultaneous first-order differential equations)
- Generation of Ordered MATLAB⁴ Code for Problem

The differential mass balances on a batch reactor yield

$$\frac{dC_A}{dt} = -k_1 C_A \quad \text{I. C. } C_A|_{t=0} = 1$$

$$\frac{dC_B}{dt} = k_1 C_A - k_2 C_B \quad \text{I. C. } C_B|_{t=0} = 0$$

$$\frac{dC_C}{dt} = k_2 C_B \quad \text{I. C. } C_C|_{t=0} = 0$$

$$k_1 = 2 \quad k_2 = 3$$

POLYMATH Solution – A Brief Look

Entry of this sample problem is accomplished within the POLYMATH full screen editor as shown in Figure 1. Note that entry is facilitated for new users by use of templates for the input of differential equations or explicit algebraic equations.

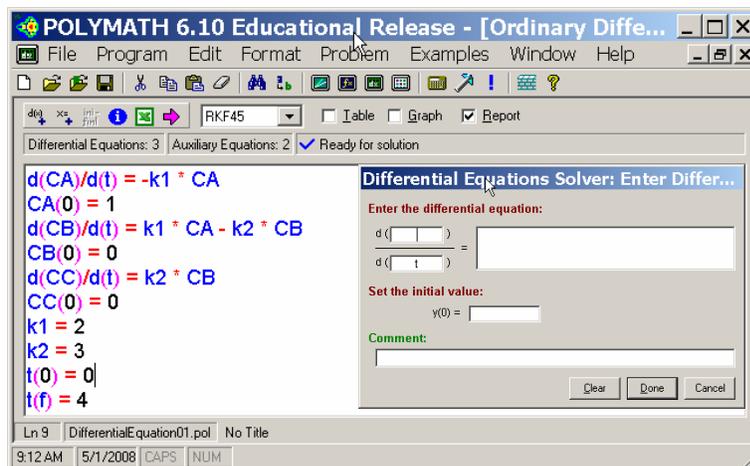


Figure 1 – Entry of Differential Equations into POLYMATH

Selection of the desired integration algorithm and the desired output followed by a mouse click on the highlighted arrow yields the numerical solution. The graph output option gives the expected result shown in Figure 2. Additional options for a Table of results and for a Report of the problem solution are not shown. The POLYMATH program can handle system of nonlinear ordinary differential equations with a variety of standard integration algorithms including those for stiff systems.

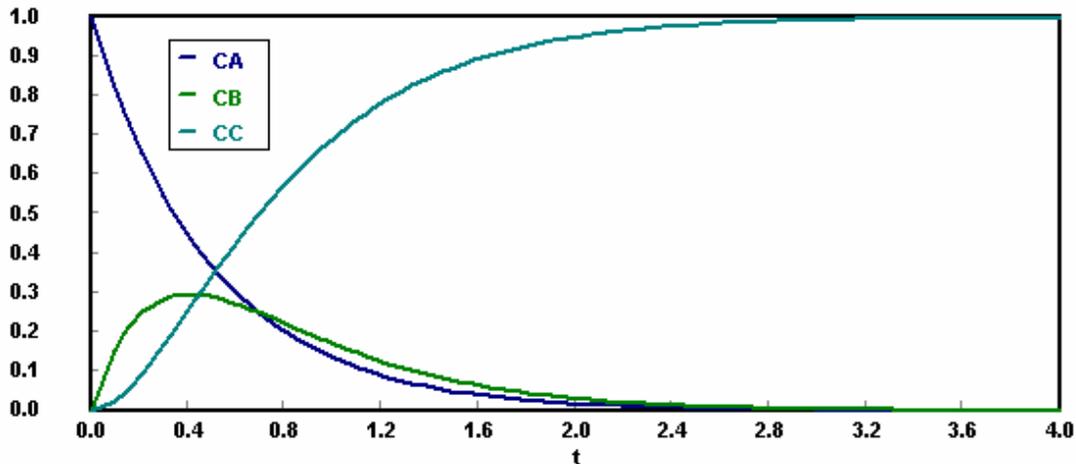


Figure 2 – Graph Output of the Differential Variables from POLYMATH

Exporting Problems from POLYMATH for Solution in Excel² – A Brief Look

Problems that can be solved completely in POLYMATH can also be automatically exported to Excel for solution. (A working spreadsheet is generated.) A POLYMATH ODE_Solver Add-In is included with POLYMATH for solving ordinary differential equations in Excel. Available Excel capabilities are used wherever they are available. For example, the provided Add-In *solver* is used to solve systems of simultaneous nonlinear equations in Excel.

The Excel solution for this sample problem is achieved by clicking the Excel icon from the POLYMATH editor. This then automatically exports the problem to an open Excel spreadsheet as shown in Figure 3. Note that all intrinsic functions and logical variables are automatically converted and placed in the Excel spreadsheet. The POLYMATH variable names and equations are shown for the convenience of the user. Since Excel does not have a differential equation solver, an Add-In, ODE_Solver.xla, is provided along with POLYMATH that will solve simultaneous ordinary differential equations. This additional software runs completely independently of POLYMATH.

The Excel solution is automatically generated in a new worksheet as shown in Figure 4. Note that a Table is given that summarizes the solution over the integration interval. Also output of the desired variables by tabulated column give the user options for use or plotting within Excel.

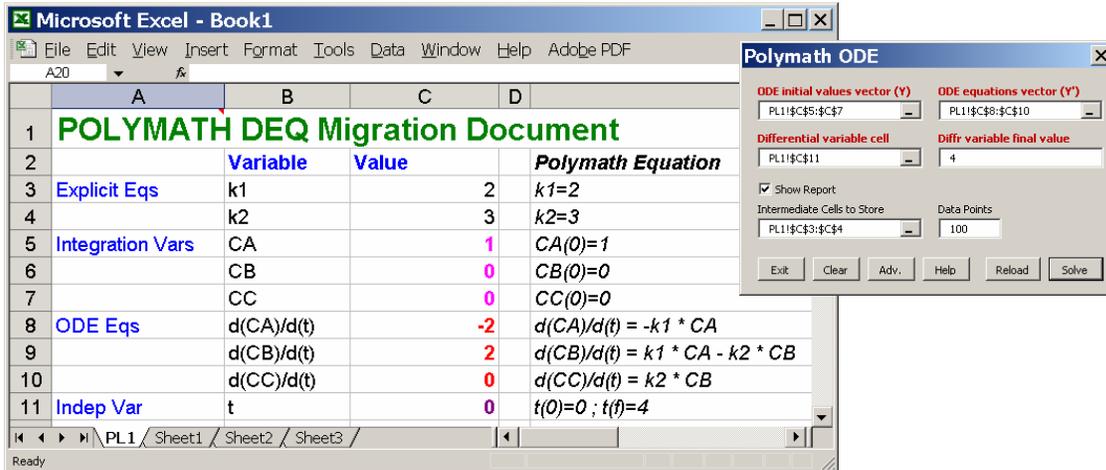


Figure 3 – Excel Spreadsheet with POLYMATH ODE_Solver Add-In

The screenshot shows a 'POLYMATH Report DEQ' worksheet with the following data:

POLYMATH Report DEQ						
Ordinary Differential Equations (RKF45).						
Calculated values of DEQ variables						
	Variable	Initial	Minimal	Maximal	Final	
6	1 t	0	0	4	4	
7	2 CA	1	0.000335	1	0.000335	
8	3 CB	0	0	0.296062	0.000659	
9	4 CC	0	0	0.999006	0.999006	
10	5 k1	2	2	2	2	
11	6 k2	3	3	3	3	
Intermediate data points						
	t	CA	CB	CC	k1	k2
15	1	0	1	0	0	2 3
16	2	0.082463	0.847957	0.134239	0.017804	2 3
17	3	0.133428	0.765783	0.191308	0.04291	2 3

Figure 4 – Worksheet Automatically Generated During Sample Problem Solution

Exporting Problems from POLYMATH to MATLAB for Solution – A Brief Look

The MATLAB solution for this sample problem is obtained by setting an option within POLYMATH that will output the problem code for MATLAB to utilize. This option leads to code which contains the translation of the intrinsic function and logical from POLYMATH into MATLAB code automatically. The generated code for this sample problem is shown in Figure 5 as is provided at the end of the POLYMATH program report.

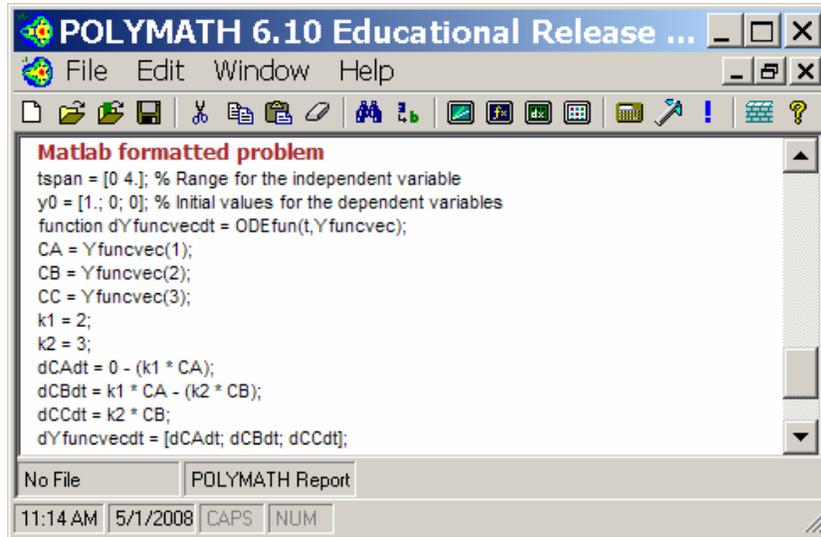


Figure 5 – POLYMATH Generated MATLAB Code

Incorporation of the generated code into the MATLAB Template for simultaneous ordinary differential equation gives the m-file given in Figure 6 where the yellow bars indicate the placement of the code generated by POLYMATH.

```

1 function MATLAB01
2 clear, clc, format short g, format compact
3 tspan = [0 4.]; % Range for the independent variable
4 y0 = [1.; 0; 0]; % Initial values for the dependent variables
5 disp(' Variable values at the initial point ');
6 disp([' t      = ' num2str(tspan(1))]);
7 disp('      y      dy/dt      ');
8 disp([y0 ODEfun(tspan(1),y0)]);
9 [t,y]=ode45(@ODEfun,tspan,y0);
10 for i=1:size(y,2)
11     disp([' Solution for dependent variable y' int2str(i)]);
12     disp(['      t      y' int2str(i)]);
13     disp([t y(:,i)]);
14     plot(t,y(:,i));
15     title([' Plot of dependent variable y' int2str(i)]);
16     xlabel(' Independent variable (t)');
17     ylabel([' Dependent variable y' int2str(i)]);
18     pause
19 end
20 %- - - - -
21 function dYfuncvecdt = ODEfun(t,Yfuncvec);
22 CA = Yfuncvec(1);
23 CB = Yfuncvec(2);
24 CC = Yfuncvec(3);
25 k1 = 2;
26 k2 = 3;
27 dCA&dt = 0 - (k1 * CA);
28 dCB&dt = k1 * CA - (k2 * CB);
29 dCC&dt = k2 * CB;
30 dYfuncvecdt = [dCA&dt; dCB&dt; dCC&dt];

```

Figure 6 – Code for MATLAB m-file

The working m-file gives both tabular results (not shown) and graphical results (partly shown in Figure 7).

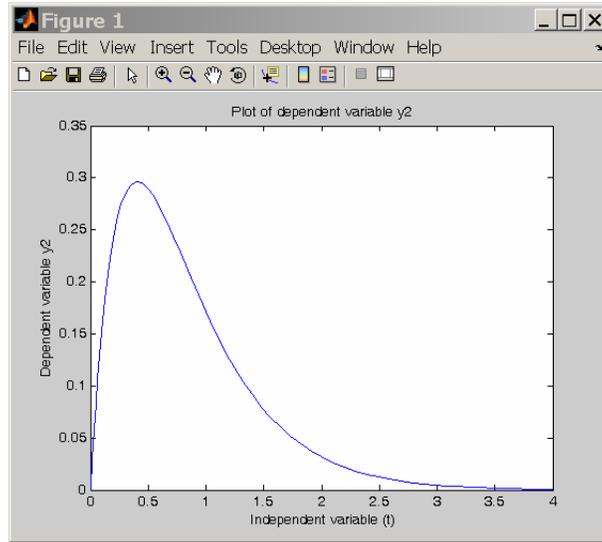


Figure 7 – Partial Graphical Results as Generated by MATLAB for Concentration of B

Integrating the Use of POLYMATH, Excel, and MATLAB

The POLYMATH software enables a programming and problem solving environment that also can utilize Excel and MATLAB as is shown in Figure 8. In this environment, the problem is first entered into POLYMATH and then can be automatically exported to Excel. From the initial POLYMATH program, the capability to generate MATLAB code enables the creation of a problem m-file.

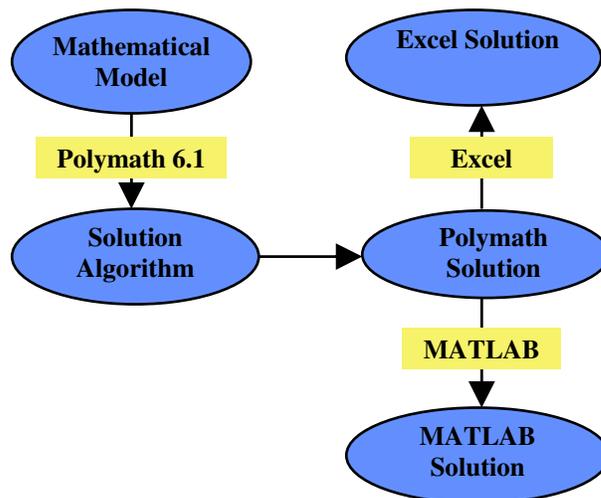


Figure 8 – Desktop Programming/Problem Solving Environment

This environment can be provided in a computer laboratory or to students and faculty for use on their own personal computers under. The POLYMATH .site license allows distribution of POLYMATH to all students, faculty, and staff plus use in all computer labs. Excel is widely available as a component of the Microsoft Office software, and this is usually available in computer labs and on individual computers. MATLAB provides inexpensive site licenses to most colleges and universities and also markets student versions.

Special Offer of POLYMATH Software to ASEE Global Symposium Participants

The authors of POLYMATH, who are engineering academics themselves, will provide all attending academics with a free site license of POLYMATH for their department or engineering college that will run through September of 2009. After that time, academic institutions in developing countries with very limited financial resources can obtain free renewals by annual application to POLYMATH Software. Institution with appropriate financial resources can purchase a site license from the CACHE Corporation that is currently costing \$200 per year. This includes the distribution to all students, faculty, and staff plus the use in all departmental computer labs. Information on this special offer of free licenses can be obtained by contacting academic@polymath-software.com.

Conclusions

- POLYMATH Software provides personal computers with extensive interactive software that can be widely used for engineering and scientific problem solving.
- The automatic export of problems from POLYMATH to Excel enables the efficient use of this spreadsheet software in the solution of a variety of problems.
- The generation of ordered MATLAB code by POLYMATH enables this high-level and programmable software to solve many problems and enable extensions to higher level capabilities where programming is involved.
- Most universities and colleges as well as personal computer owners already have Excel available for use and interaction with POLYMATH.
- Many universities and colleges have site licenses for MATLAB that provide this software to students, faculty, and staff.
- The special offer from Polymath Software and the CACHE Corporation will enable free use and evaluation of the software by academic departments of the ASEE Global Symposium participants through September of 2009.
- Future use of an inexpensive POLYMATH site license can be purchased by departments from the CACHE Corporation. This allows wide distribution of the software to individual and use in computer labs.
- Future continuing use of site licenses by departments in developing countries with limited financial resources will be enabled at no cost by annual request to Polymath Software.

References

1. CACHE Corporation, <http://www.cache.org/>. CACHE, which stands for Computer Aids for Chemical Engineering, is a not-for-profit organization whose purpose is to promote cooperation among universities, industry and government in the development and distribution of computer-related and/or technology-based educational aids for the chemical engineering profession. CACHE was initially sponsored by the Commission on Education of the National Academy of Engineering and funded by the National Science Foundation. The current Executive Officer of CACHE is Professor Thomas F. Edgar of the University of Texas at Austin.
2. Polymath Software, <http://www.polymath-software.com/>. The various POLYMATH programs allow the user to apply effective numerical analysis techniques during interactive problem solving on personal computers. The CACHE Corporation provides site licenses for POLYMATH to colleges and universities.
3. Microsoft Corporation, <http://www.microsoft.com>. Windows 95, Vista, Excel, and Microsoft Office are products and trademarks of the Microsoft Corporation.
4. MATLAB is a product and trademark of The MathWorks, Inc., <http://www.mathworks.com>.