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Chebyshev Orthogonal Collocation Technique to Solve Transport Phenomena Problems With Matlab® and Mathematica©

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ABSTRACT: We present in this pedagogical paper an alternative numerical method for the resolution of transport phenomena problems encountered in the teaching of the required course on transport phenomena in the graduate chemical engineering curricula. Based on the Chebyshev orthogonal collocation technique implemented in Matlab® and Mathematica©, we show how different rather complicated transport phenomena problems involving partial differential equations and split boundary value problems can now readily be mastered. A description of several sample problems and the resolution methodology is discussed in this paper. The objective of the incorporation of this approach is to develop the numerical skills of the graduate students at King Fahd University of Petroleum & Minerals (KFUPM) and to broaden the extent of transport-phenomena problems that can be addressed in the course. We noted with satisfaction that the students successfully adopted this numerical technique for the resolution of problems assigned as term projects. Comput Appl Eng Educ 9999:1–10, 2014; View this article online at wileyonlinelibrary.com/journal/cae; DOI 10.1002/cae.21612

Keywords: transport phenomena; orthogonal collocation; Chebyshev; Matlab®; Mathematica©

INTRODUCTION

The teaching of Transport Phenomena and Numerical Methods is typical of graduate programs in chemical engineering. We need not elaborate on the different phases in the teaching of the Numerical Methods course; however, it is fair to suggest that there are three distinct phases: (1) development of Fortran programs [1,2]; (2) application of IMSL codes; and (3) application of commercial software codes. The great revolution in computational power has allowed most users to focus on the third phase, where software codes, such as Matlab, Mathcad, or Mathematica can be used to attack a variety of engineering problems in reaction analysis and transport phenomena. The integration of such software codes in chemical engineering education, both at the undergraduate and graduate levels, has been discussed in the literature in several articles; see for example, Loughlin and Shaikh [3] and Parulekar [4]. Further examples for solutions of typical problems in Transport Phenomena using different numerical approaches and appropriate software can be found in Refs. [5–14].

In the present paper, we address ourselves to the numerical solution of highly nonlinear problems in the graduate-level Transport Phenomena course. As described in the syllabus (see Appendix A), the graduate-level transport phenomena course taught at KFUPM uses the textbook written by Bird et al. [15]. A short mathematical introduction on how to use tensors, gradients (Appendix A of BSL), etc. is given during the first week of instruction. Later, the instructor reviews the three constitutive equations (Newton's law of viscosity, Fourier's law, and Fick's law; Chapters 1, 9, and 17 of BSL). Shell momentum, heat and

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mass balances are rapidly reviewed (Chapters 2, 10, and 18). Then, the equation of motion (chapter 3 of BSL) is thoroughly taught. The equations of change for non-isothermal and multi-component systems are also introduced (Chapters 11 and 19 of BSL). Finally, problems involving more than one independent variable are treated with emphasis on the analytical methods of solution such as the separation of variables and the similarity transform techniques (Chapter 4, 12, and 20 of BSL).

In the graduate-level transport phenomena course at KFUPM, several performance assessment tools are used by the instructor. These include bi-weekly assignments, midterm and final examinations, as well as term projects. In the term projects, each student is asked to solve a transport-phenomena problem using Matlab® or Mathematica© and the Chebyshev orthogonal collocation method.

In the fall semester of 2013, these term project problems (each problem assigned to a group of two students) have involved

- transient Couette flow,
- transient Poiseuille flow,
- steady-state flow of non-Newtonian fluids in a pipe,
- unsteady-state evaporation of liquids,
- 1-D transient heat conduction in a cylinder,
- the Falkner–Skan Equation,
- 1-D steady-state heat diffusion with temperature-depend heat conductivity, and finally,
- unsteady state convection-diffusion.

A set of seven typical transport phenomena problems is discussed in the present paper. We begin with a short description of the Chebyshev orthogonal collocation method and illustrate the solution technique through two examples. We conclude with our experience in teaching advanced topics in chemical engineering using the computational tools described here.

THE CHEBYSHEV ORTHOGONAL COLLOCATION METHOD

The Derivative Matrix

In the discrete Chebyshev–Gauss–Lobatto orthogonal collocation method, the grid points are defined by

$$y_j = \cos\frac{j\pi}{N}, \quad j = 0, \ldots, N \tag{1}$$

and represent the locations of the extrema of the first kind Chebyshev polynomials, $T_N(x)$. The $(N+1)\times(N+1)$ Chebyshev derivative matrix D at the quadrature points is [16–18]:

$$D = (d_{jk})_{0\le j,k,\le N} \tag{2}$$

with

$$\begin{cases} d_{00} = \dfrac{2N^2+1}{6} \\ d_{NN} = \dfrac{2N^2+1}{6} \\ d_{jj} = -\dfrac{y_j}{2(1-y_j^2)} \text{ for } 1 \le j \le N\text{-}1 \end{cases}$$

For $0 \le j,\ k \le N$ with $j \ne k$, the element d_{jk} writes

$$d_{jk} = \frac{c_j(-1)^{j+k}}{c_k(y_j - y_k)}$$

with

$c_m = 1$ for $1 \le m \le N-1$ and $c_0 = c_N = 2$.

If v is the vector formed by the values of the function $u(y)$ at the locations $y_j, j = 0, \ldots, N$ the values of the approximations v' and v'' of the derivates u' and u'' of u at the grid points y_j are calculated as follows:

$$v' = Dv; \quad v'' = D^2 v$$

where D is the differentiation matrix. The Mathematica© code for building D is given in Appendix B. A similar code, this time based on Matlab®, can be found in the textbook by Trefethen [18].

ILLUSTRATION OF THE CHEBYSHEV COLLOCATION TECHNIQUE USING MATLAB® OR MATHEMATICA© THROUGH TWO SIMPLE EXAMPLES

A Simple Split Boundary Value Problem

Consider the following nonlinear boundary value problem encountered in a graduate-level applied mathematics course:

$$uu' - u'' = 1 \tag{3}$$

with the boundary conditions

$$u(-1) = 0, \quad u(1) = 2.$$

It is possible to find the solution $u(-1 \le y \le 1)$ at the locations $y_j = \cos(j\pi/N)$ for $j = 0, \ldots, N$, by solving the following system of $(N+1)$ nonlinear algebraic equations:

$$\begin{cases} u_j\left(\sum\limits_{k=0}^{N} d_{jk}u_k\right) - \sum\limits_{k=0}^{N} b_{jk}u_k = 1,\ j = 1, \ldots, (N-1) \\ u_0 = 2 \\ u_N = 0 \end{cases} \tag{4}$$

where $(d_{jk})_{0\le j,k\le N}$ are the elements of the derivation matrix D given in the previous section and $(b_{jk})_{0\le j,k\le N}$ the elements of $D^2 = D{\cdot}D$. Such system of nonlinear algebraic equations is readily solved using Mathematica© and Matlab® built-in functions **FindRoot** and **fsolve** respectively. For $N = 20$ the solution, u, at the collocation points, $y_j, j = 0, \ldots, 20$, is given in Table 1 and plotted in Figure 1. We intentionally represent for all the treated cases the calculation results in graphical and table forms especially for readers who want to rework the problems and are interested not only in solution trends but also in exact numerical solution of these potential benchmark problems in transport phenomena processes. A solution of this problem can be found using the shooting technique. The data obtained using this later method, are also given in Table 1 for comparison purposes.

A Simple Partial Differential Equation

Consider the following partial differential equation (PDE):

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial y^2} \tag{5}$$

with the initial and boundary conditions

$$u(t=0,y) = 1$$
$$u(t,y=0) = 0$$
$$u(t,y=1) = 0$$

Table 1 Values at the Collocation Points of the Solution of the Nonlinear Boundary Value Problem of Illustration 1

j	y_j	u_j[a]	u_j[b]
0	1.0000	2.0000	2.[Q3]
1	0.9877	1.9837	1.9836
2	0.9511	1.9366	1.9365
3	0.8910	1.8634	1.8634
4	0.8090	1.7704	1.7704
5	0.7071	1.6634	1.6634
6	0.5878	1.5471	1.5470
7	0.4540	1.4243	1.4243
8	0.3090	1.2969	1.2969
9	0.1564	1.1656	1.1656
10	0.0000	1.0310	1.0309
11	−0.1564	0.8938	0.8937
12	−0.3090	0.7552	0.7551
13	−0.4540	0.6170	0.6170
14	−0.5878	0.4822	0.4822
15	−0.7071	0.3545	0.3544
16	−0.8090	0.2385	0.2385
17	−0.8910	0.1399	0.1398
18	−0.9511	0.0642	0.0641
19	−0.9877	0.0164	0.0163
20	−1.0000	0	-2.4087×10^{-21}

[a]Chebyshev collocation.
[b]Shooting method.

This is the well-known one-dimensional diffusion equation. It is possible to find the solution $u(t,\ 0 \leq y \leq 1)$ at $y_j = (1 + \cos(j\pi/N))/2$, $j = 0, \ldots, N$, by solving the following system of $(N+1)$ differential algebraic equations (DAEs):

$$\begin{cases} u'_j(t) = 4\sum_{k=0}^{N} b_{jk}u_k(t),\ j = 1, \ldots, N-1 \\ u_0(t) = 0 \\ u_N(t) = 0 \end{cases} \tag{6}$$

where $D^2 = D \cdot D = (b_{jk})_{0 \leq j,k \leq N}$ is the square of the derivative matrix, D is the initial conditions for the DAEs are $u_j(t=0) = 1$ for $j = 0, \ldots, N$. Such system of differential algebraic equations is readily solved using Mathematica© and Matlab® built-in functions **NDSolve** and **ode15s**, respectively. The solution, u, at $t = 0.0126$ and at the collocation points, y_j, $j = 0, \ldots, N$ for $N = 20$ is given in Table 2 and plotted in Figure 2. This transport problem admits an analytical solution derived using the separation of variable technique given by:

$$u(t,y) = \sum_{n=1}^{\infty} \frac{2}{n\pi}(1 - \cos(n\pi))e^{-n^2\pi^2 t}\sin(n\pi x). \tag{7}$$

The data obtained, using the analytical solution, are also presented in Table 2 for comparison purposes.

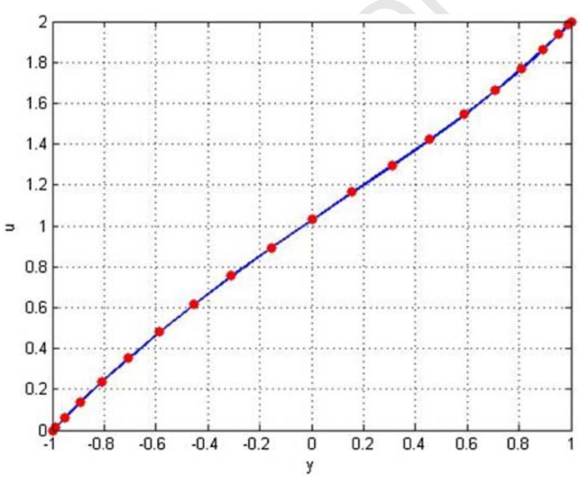

Figure 1 Solution of the nonlinear boundary value problem of illustration 1. (Red dots: Chebyshev collocation, blue curve: shooting method[Q4].) [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

CASE STUDIES

The Arnold Problem

Consider as a first case the unsteady evaporation of a liquid A in non-diffusing gas B. The migration of particles A in the gas phase is described by the equation [19]:

$$\frac{\partial c_A}{\partial t} = D_{AB}\frac{\partial^2 c_A}{\partial z^2} + \left[\frac{D_{AB}}{1 - (c_{A0}/c_t)}\left(\frac{\partial c_A}{\partial z}\right)_{z=0}\right]\frac{\partial c_A}{\partial z} \tag{8}$$

where D_{AB} is the gas diffusion coefficient, c_{A0}, the interfacial gas-phase concentration, z, the vertical gas phase position and $c_t = c_A + c_B$.

The initial and boundary conditions for this problem are:

$t = 0, \quad c_A(z,0) = 0$

$z = 0, \quad c_A(0,t) = c_{A0}$(Interface liquid–vapor equilibrium condition)

$z = \infty, \quad c_A(\infty,t) = 0$

Equation (8) has an analytical solution:

$$\frac{c_A(\xi)}{c_{A0}} = \frac{1 - \text{erf}(\xi - \phi)}{1 + \text{erf}(\phi)}, \tag{9}$$

Table 2 Values at the Collocation Points of the Solution of the Diffusion Equation of Illustration 2 at $t = 0.0126$

j	y_j	u_j[a]	u_j[b]
0	1.0000	0	0.[Q5]
1	0.9938	0.0307	0.0309
2	0.9755	0.1218	0.1225
3	0.9455	0.2670	0.2686
4	0.9045	0.4500	0.4525
5	0.8536	0.6407	0.6437
6	0.7939	0.8029	0.8058
7	0.7270	0.9124	0.9145
8	0.6545	0.9693	0.9704
9	0.5782	0.9914	0.9918
10	0.5000	0.9965	0.9967
11	0.4218	0.9914	0.9918
12	0.3455	0.9693	0.9704
13	0.2730	0.9124	0.9145
14	0.2061	0.8029	0.8058
15	0.1464	0.6407	0.6437
16	0.0955	0.4500	0.4525
17	0.0545	0.2670	0.2686
18	0.0245	0.1218	0.1225
19	0.0062	0.0307	0.03093
20	0	0	0.

[a]Chebyshev collocation.
[b]Separation of variables.

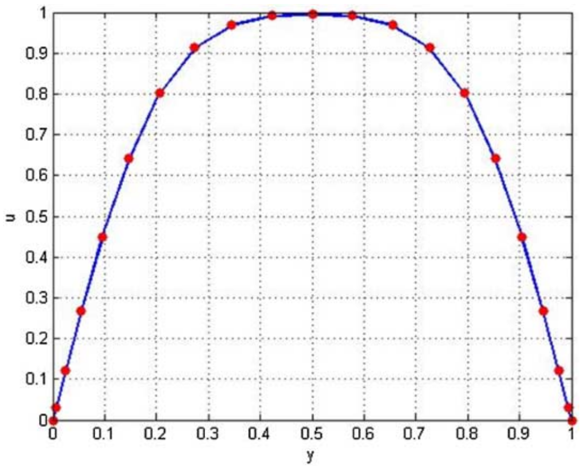

Figure 2 Solution of the diffusion equation of illustration 2. (Red dots: Chebyshev collocation, blue curve: analytical solution.) [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

where $\xi = \left(z/\sqrt{4D_{AB}t}\right)$ and ϕ a solution of the nonlinear equation:

$$\phi = \frac{1}{\sqrt{\pi}} \frac{c_{A0}/c_t}{(1-(c_{A0}/c_t))} \frac{e^{-\phi^2}}{(1+\mathrm{erf}(\phi))}. \tag{10}$$

The numerical solution of Equation (8) using a Mathematica© implementation of the Chebyshev orthogonal collocation involves using **NDSolve** to solve the system of $(N+1)$ DAEs:

$$\begin{aligned} c_{A,N}(t) &= c_{A0} \\ c'_{A,j}(t) &= D_{AB}\left(\frac{2}{L}\right)^2\left(\sum_{k=0}^{N} b_{jk}c_{A,k}(t)\right) + \frac{D_{AB}}{1-(c_{A0}/c_t)}\left(\frac{2}{L}\right) \\ &\quad \times \left(\sum_{k=0}^{N} d_{0k}c_{A,k}(t)\right)\left(\frac{2}{L}\right)\left(\sum_{k=0}^{N} d_{jk}c_{A,k}(t)\right), \\ \text{for} \quad j &= 1, \ldots, N-1 \\ c_{A,0}(t) &= 0 \end{aligned}$$

where $(d_{jk})_{0\le j,k\le N}$ are the elements of the derivative matrix D, $(d_{jk})_{0\le j,k\le N}$, the elements of its square, $D^2 = D{\cdot}D$, and $L = 8$.

The initial conditions for the DAEs are $c_{A,j}(z,0) = 0$ for $j = 0, \ldots, N$.

The solution $c_A(t,\ 0 \le z \le L = 8)$ is found at the grid points $z_j = L(1+\cos(j\pi/N))/2$ for $j = 0, \ldots, N$.

The numerical solution, $c_A(z,\ t)$, thus obtained (red dots in Fig. 3) can be compared to the analytical solution represented by the blue curve on the same figure. Excellent agreement between both solutions is observed.

The built-in Mathematica© command **Manipulate** allows students to create interactive programs with sliders, check boxes, controls, etc. Here, one can vary the values of t, D_{AB}, c_{A0} as well as the number of the Chebyshev collocation points, $(N+1)$, and instantaneously see the effect of variables and parameters.

Unsteady-State Convection-Diffusion Problem

Consider the unsteady 1-D convection-diffusion problem described by the equation:

$$\frac{\partial c}{\partial t} = D_f \frac{\partial^2 c}{\partial x^2} - v\frac{\partial c}{\partial x}, \tag{11}$$

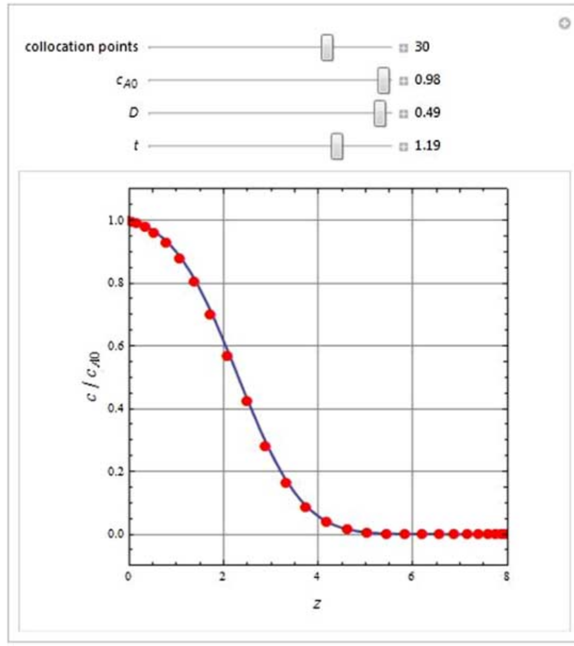

Figure 3 Composition profile for the Arnold problem. (Red dots: Chebyshev collocation, blue curve: analytical solution.) [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

where D_f is the diffusion coefficient, v the velocity, c the concentration of the diffusing species, and x is the position in the direction of flow.

With the following initial and boundary conditions:

$$\begin{aligned} t &= 0, \quad c(x,0) = 0, \\ x &= 0, \quad c(0,t) = 1, \\ x &= \infty, \quad c(\infty,t) = 0. \end{aligned}$$

Equation (11) has an analytical solution that can be readily be found using Laplace transforms:

$$c(x,t) = \frac{1}{2}\left(\mathrm{erfc}\left[\frac{x-vt}{2\sqrt{Dt}}\right] + e^{(vx)/D}\mathrm{erfc}\left[\frac{x+vt}{2\sqrt{Dt}}\right]\right). \tag{12}$$

In Figure 4 the evolution of the concentration $c(x,\ t)$ represented by the analytical solution (blue curve) and the numerical solution $c(t,\ 0 \le x \le L = 10)$ obtained using the implementation of the Chebyshev orthogonal collocation in Mathematica© (red dots) are compared. Again, an excellent agreement between the two solutions is observed.

As noted in the previous case study, the built-in Mathematica© command **Manipulate** allows creating interactive numerical solutions of Equation (11) by varying the values of t, D_f, v as well as the number of the Chebyshev collocation grid points $(N+1)$.

The Falkner–Skan Equation

The flow past a wedge at an angle of attack β from some uniform velocity field U_0 is governed by a non-linear ODE known as the Falkner–Skan equation [20], named after V. M. Falkner and S. W. Skan [21]:

$$f^{(3)} = ff^{(2)} + \beta(1-(f')^2) = 0 \tag{13}$$

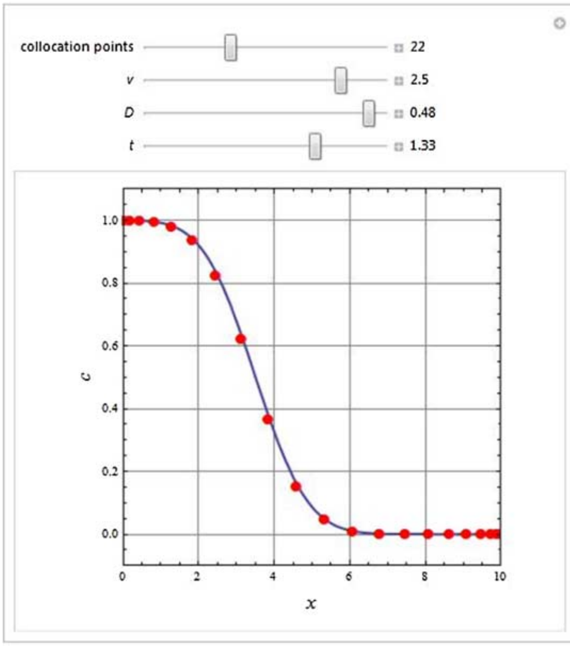

Figure 4 Composition profile for the unsteady-state convection-diffusion problem. (Red dots: Chebyshev collocation, blue curve: analytical solution.) [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

with the limit conditions

$$f(0) = f'(0) = 0 \quad \text{and} \quad f'(\infty) = 1.$$

Equation (13) admits only a numerical solution which requires the application of an appropriate numerical algorithm (shooting method, Chebyshev orthogonal collocation, etc.)

Figure 5 shows the velocity or f' obtained with the help of Matlab® for a wedge angle $\beta = (\pi/4)$. Applying the shooting technique leads to the blue curve while the red dots represent the velocity obtained using the Chebyshev orthogonal collocation method by solving a system of $(N+1)$ nonlinear algebraic equations using the built-in command **fsolve**.

The equations system is the following

$$\begin{cases} \sum_{k=0}^{N} d_{0k} f_k = 1 \\ \sum_{k=0}^{N} d_{Nk} f_k = 0 \\ f_N = 0 \\ \left(\frac{2}{L}\right)^3 \left(\sum_{k=0}^{N} e_{jk} f_k\right) + \left(\frac{2}{L}\right)^2 \left(\sum_{k=0}^{N} b_{jk} f_k\right) + \beta\left(1 - \left(\left(\frac{2}{L}\right)\left(\sum_{k=0}^{N} d_{jk} f_k\right)^2\right)\right) = 0 \\ \text{for } j = 1, \ldots, N-2 \end{cases}$$

where $(d_{jk})_{0\leq j,k\leq N}$ are the elements of the derivative matrix D, $(b_{jk})_{0\leq j,k\leq N}$, the elements of its square, $D^2 = D{\cdot}D$, and $(e_{jk})_{0\leq j,k\leq N}$ those of its cube $D^3 = D{\cdot}D{\cdot}D$.

The function values $f(0 \leq y \leq L = 4)$ are found at the grid points $y_j = L(1+\cos(j\pi/N))/2$, for $j = 0, \ldots, N$.

The well-known Blasius equation (flow past a flat plate with a wedge angle, $\beta = 0$) appears as a particular case in this study.

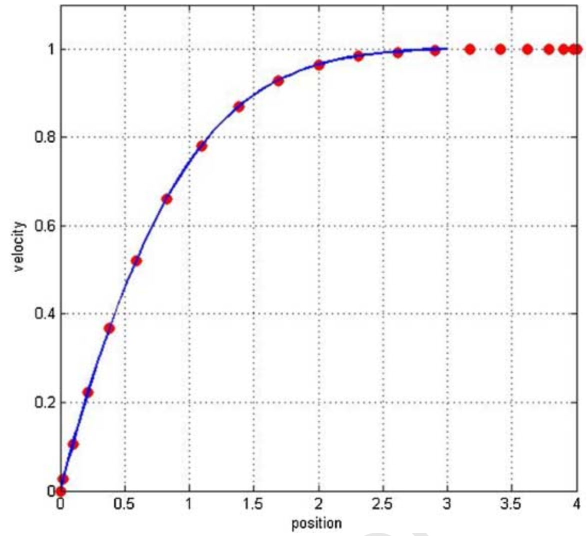

Figure 5 Velocity profile for flow past a wedge ($\beta = (\pi/4)$). (Red dots: Chebyshev collocation, blue curve: shooting technique.) [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Planar stagnation flow is also found by setting the wedge attack angle $\beta = \pi$.

Pipe Flow of Power-Law and Carreau fluids

A non-Newtonian fluid has a viscosity that changes with the applied shear force. For a Newtonian fluid (such as water), the viscosity is independent of how fast it is stirred, but for a non-Newtonian fluid the viscosity is dependent on the stirring rate. It gets either easier or harder to stir faster for different types of non-Newtonian fluids. Different constitutive equations, giving rise to various models of non-Newtonian fluids, have been proposed in order to express the viscosity as a function of the strain rate.

In power-law fluids, the relation

$$\mu = \kappa \dot{\ } \gamma^{n-1} \tag{14}$$

is assumed, where n is the power-law exponent and k is the power-law consistency index. Dilatant or shear-thickening fluids correspond to the case where the exponent in this equation is positive, while pseudo-plastic or shear-thinning fluids are obtained when $n < 1$. The viscosity decreases with strain rate for $n < 1$, which is the case for pseudo-plastic fluids (also called shear-thinning fluids). On the other hand, dilatant fluids are shear thickening. If $n = 1$, the Newtonian fluid behavior can be recovered. The power-law consistency index is chosen to be $k = 1.5 \times 10^{-5}$. For the pseudo-plastic fluid, the velocity profile is flatter near the center, where it resembles plug flow, and is steeper near the wall, where it has a higher velocity than the Newtonian fluid or the dilatant fluid. Thus, convective energy transport is higher for shear-thinning fluids when compared to shear-thickening or Newtonian fluids. For flow in a pipe of a power-law fluid, an analytical expression is available [22,23]. According to the Carreau model for non-Newtonian fluids, first proposed by Pierre Carreau,

$$\mu = (\dot{\ }\gamma) - \mu_\infty = (\mu_0 - \mu_\infty)(1 + \lambda^2 \dot{\ } \gamma^2)^{((n-2)/2)} \tag{15}$$

For $\lambda\gamma \ll 1$, this reduces to a Newtonian fluid with $\mu = \mu_0$. For $\lambda\gamma \gg 1$, we obtain a power-law fluid with $\mu = \kappa\,\dot{\gamma}^{n-1}$.

The infinite-shear viscosity μ_∞ and the zero-shear viscosity μ_0 of the Carreau fluid are taken equal to 0 and 2.04×10^{-3}, respectively. The relaxation parameter λ is set equal to 0.2. For the flow of a Carreau fluid in a pipe, only numerical solutions are available. The velocity profile versus radial position is obtained for the steady-state laminar flow of power-law and Carreau fluids in a pipe. The pipe radius is $R = 1$ and the applied pressure gradient is $((\Delta P)/L) = 1$. For both the power-law and Carreau fluids, the red dots represent the solutions obtained using the Chebyshev collocation technique (see Fig. 6a and b). The velocity profile for a power-law fluid (the blue curve) is obtained from the analytical solution given by Binous [22] and Wilkes [23]:

$$v(r) = \left(\frac{\Delta P}{2L\kappa}\right)^{1/n} \frac{R^{1+1/n} - r^{1+1/n}}{1 + 1/n}. \tag{16}$$

The velocity profile for a Carreau fluid (the blue curve) is obtained using the shooting technique and the built-in Mathematica function **NDSolve**. For both fluids, you can vary the exponent.

The Chebyshev orthogonal collocation technique requires the solution of a system of $(N+1)$ nonlinear algebraic equations. Here, the Mathematica© methodology is based on the usage of the built-in command **FindRoot**.

Free Convection Past an Isothermal Vertical Plate

Consider the free convection past a vertical flat plate or wall maintained at a constant temperature T_w with $T_w > T_\infty$, where T_∞ is the fluid temperature far from the wall.

The governing equations for such a problem in steady state [20,24] are:

$$\begin{cases} F^{(3)} + 3FF' - 2(F')^2 + \Theta = 0 \\ \Theta^{(2)} + 3\mathrm{Pr}F\Theta' = 0 \\ \text{with the B.C.} \\ F(0) = F'(0) = 0 \\ F'(\infty) = 0 \\ \Theta(0) = 1; \Theta(\infty) = 0 \end{cases} \tag{17}$$

where $\Theta = ((T - T_\infty)/(T_w - T_\infty))$ is the dimensionless temperature, $\mathrm{Pr} = (\nu/\alpha)$ the Prandtl number (a dimensionless number giving the rate of viscous momentum transfer relative to heat conduction), and F is the modified stream function

$$F(\eta) = \frac{\psi}{4\nu[(g\beta(Tw - T\infty))/(4\nu^2)]^{1/4} x^{3/4}}$$

of the similarity variable η

$$\eta = \left[\frac{Gr_x}{4}\right]^{1/4} \frac{y}{x}$$

The derivative F' of F is proportional to the fluid velocity. $Gr_x = ((g\beta\Delta T x^3)/\nu^2)$ is the Grashof number. To solve this split boundary value problem one has to apply an appropriate numerical procedure such as the shooting and/or relaxation technique. In this study we make use of the Chebyshev orthogonal collocation method that we implemented in Mathematica© and—for comparison purposes—the classical shooting technique. The obtained temperature and velocity profiles versus η for $\mathrm{Pr} = 8$

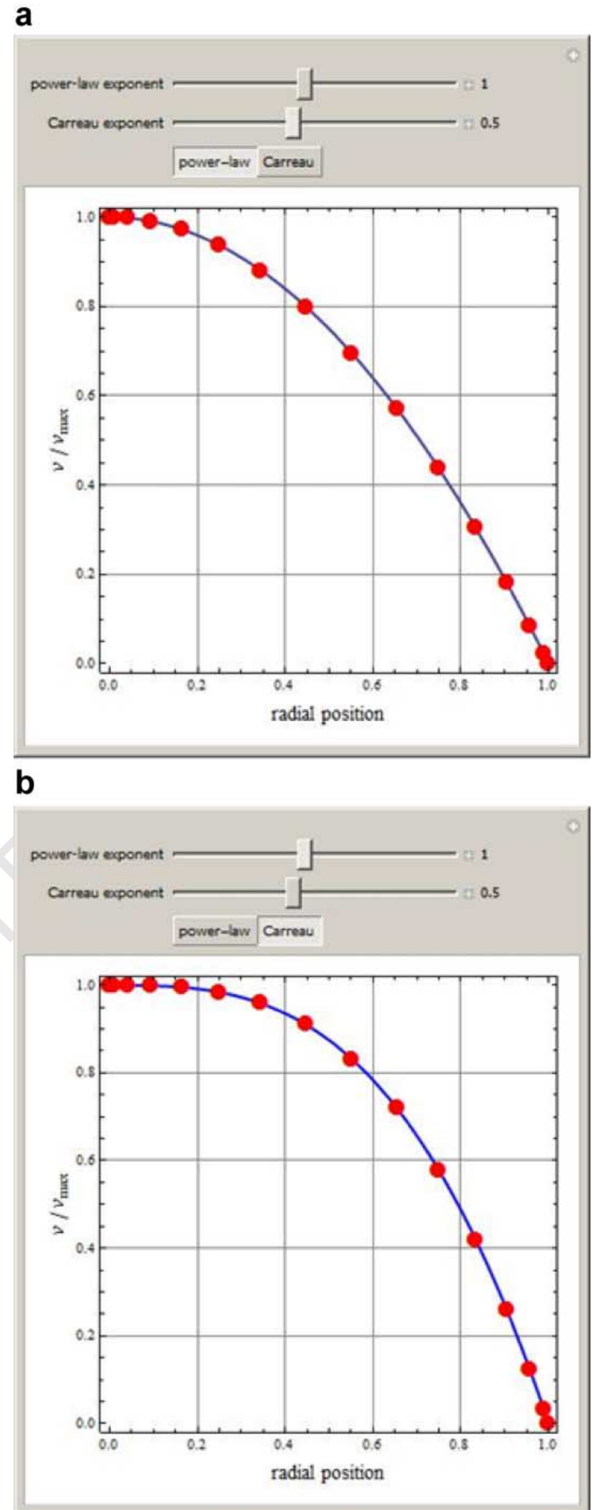

Figure 6 Velocity profile for (a) the power-law fluid and (b) the Carreau fluid. (Red dots: Chebyshev collocation, blue curve a: analytical solution, blue curve b: shooting method.) [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

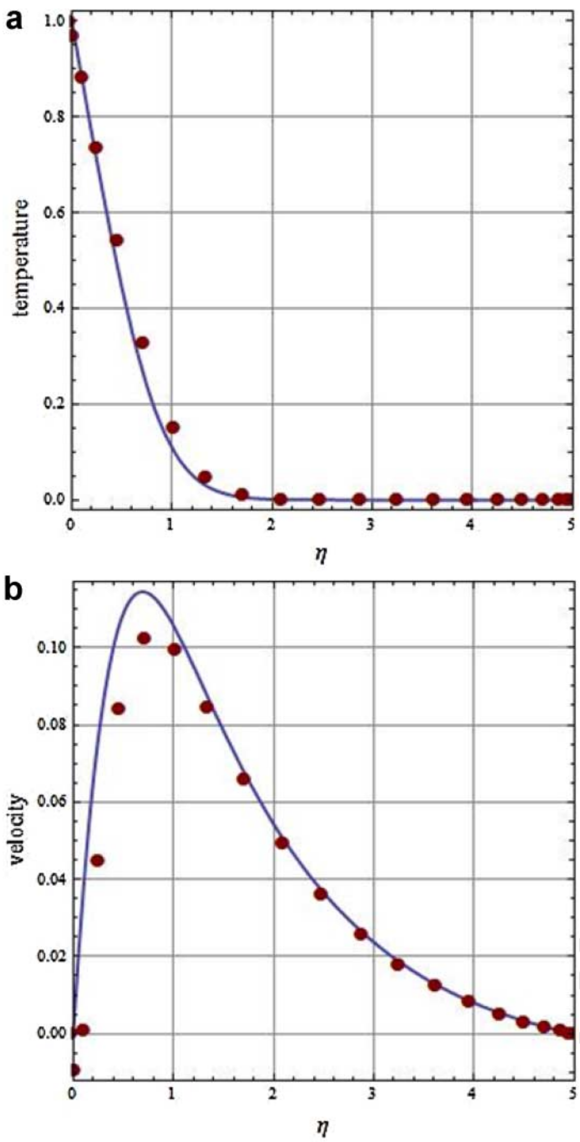

Figure 7 (a) Temperature profile and (b) velocity profile for free convection past an isothermal vertical plate in the case of $\mathrm{Pr} = 10$. (Red dots: Chebyshev collocation, blue curve: shooting technique.) [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

are represented in Figure 7a and b as red dots for the results of the Chebyshev integration approach and blue curves for the shooting method. The Chebyshev collocation procedure requires the solution of a system of $2(N+1)$ nonlinear algebraic equations using **FindRoot** in Mathematica©.

As can be noted, only qualitative agreement is obtained for the velocity profile using the shooting and the orthogonal collocation approach. One however can verify that if the Prandtl number Pr is reduced, the dimensionless temperature curve extends farther away from the wall as an indication of higher rates of heat conduction.

Start-Up of Poiseuille Flow in a Newtonian Fluid

The governing equation, in dimensionless form, for Poiseuille flow for a Newtonian fluid in a tube is given by:

$$\frac{\partial v}{\partial \tau} = 4 + \frac{1}{\xi}\frac{\partial}{\partial \xi}\left(\xi \frac{\partial v}{\partial \xi}\right), \tag{18}$$

where the dimensionless time is $\tau = ((t\nu)/R^2)$, the dimensionless radial position, $\xi = (r/R)$ and the dimensionless velocity, $v = ((V_z(r))/V_{z\,\max})$.

The boundary and initial conditions are:

$$v(\xi = 1, t) = 0,$$
$$\frac{\partial v}{\partial \xi}(\xi = 0, t) = 0,$$
$$v(\xi, t = 0) = 0.$$

$\nu = (\mu/\rho)$ is the kinematic viscosity with μ the fluid's viscosity and ρ, its density. The radius of the pipe is R, and $v_{z,\max} = -(1/4\mu)(\partial p/\partial z)R^2$ is the velocity at the center of the pipe at steady state. Figure 8 depicts the velocity profile obtained using Matlab® at $\tau = 0.1359$. Here one has to solve a system of DAEs using the built-in Matlab® command **ode15s**.

This problem admits an analytical solution given by:

$$v = \frac{V_z(r)}{V_{z,\max}} = \left(1 - \left(\frac{r}{R}\right)^2\right) - \sum_{k=1}^{\infty} A_k J_0\left(\lambda_k \frac{r}{R}\right) e^{((\nu(\lambda_k)^2)/R^2)t}$$

where

$$A_k = \frac{2}{(R^2 J_1(\lambda_k))^2} \int_0^R r J_0\left(\lambda_k \frac{r}{R}\right)(R^2 - r^2)\,\mathrm{d}r$$

and λ_k are the roots of the zeroth order Bessel function of the 1st kind (i.e., $J_0(\lambda_k) = 0$).

Table 3 gives a list of these values and Table 4 shows a comparison between the analytical solution (truncated up to $k = 7$) and our Chebyshev numerical solution.

Transient Couette Flow

This aim of this section is to show how the Couette flow in a slot develops. Initially the fluid and both walls are stationary. To start

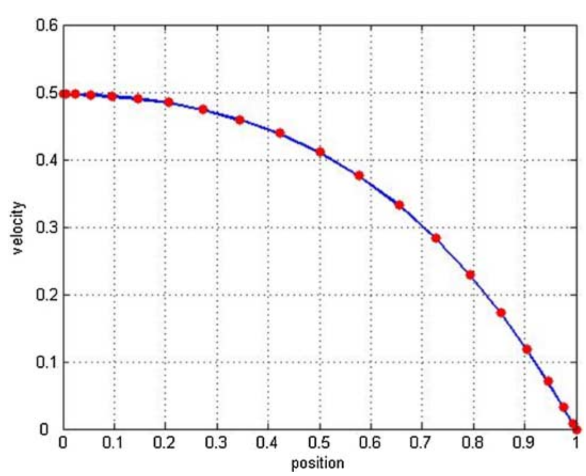

Figure 8 Velocity profile of a Poiseuille flow in a Newtonian fluid at $\tau = 0.1359$. (Red dots: Chebyshev collocation, blue curve: analytical solution.) [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Table 3 The Seven First Values of the Zeroth of J_0

k	λ_k
1	2.4048
2	5.5201
3	8.6537
4	11.7915
5	14.9309
6	18.0711
7	21.2116

the flow the lower wall is brought to a constant velocity, $u(0) = U = 1$ m/s.

The momentum equation and the no-slip boundary condition are:

$$\frac{\partial u}{\partial t} = v \frac{\partial^2 u}{\partial y^2} \tag{19}$$

and $u(1) = 0$ where v is the kinematic viscosity.

The steady-state solution is the linear velocity profile given by $u(y) = U(1 - y)$. The analytical solution of Equation (19) can be found by applying the separation of variables technique [25]:

$$u(t, y) = U(1 - y) - \frac{2}{\pi} U \sum_{k=1}^{\infty} \frac{1}{k} \sin(k\pi y) \mathrm{e}^{-k^2 \pi^2 vt}$$

Using Matlab®, we plot in Figure 9 the velocity profile at $t = 1.1255$ and $v = 0.1$. Here also one has to solve a system of DAEs using the built-in Matlab® command **ode15s**. A comparison between the numerical and analytical results (truncated up to $k = 100$) for $t = 0.1255$ and $v = 0.1$ is given in Table 5. For very small kinematic viscosities, the response is slower. This result is to be expected since the momentum transport is governed here solely by molecular momentum exchange, characterized by the kinematic viscosity (unit is cm^2/s) which is just like molecular diffusion and heat conduction in gases a very slow process.

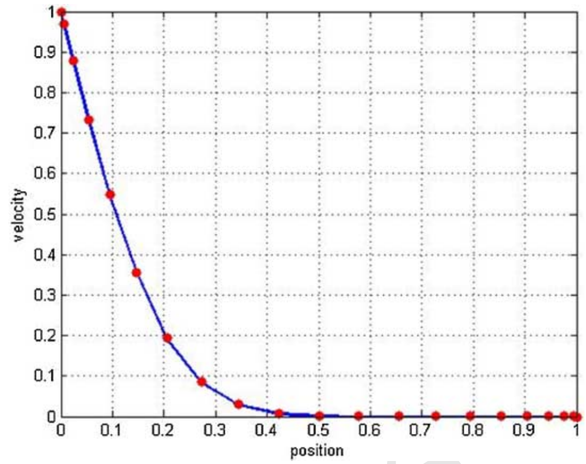

Figure 9 Velocity profile of a Couette flow of a Newtonian fluid at ($t = 0.1255$; $v = 0.1$) (Red dots: Chebyshev collocation, blue curve: analytical solution.) [Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

CONCLUDING REMARKS

In this paper, we have described how two software packages have been gainfully employed in conjunction with the orthogonal-collocation technique in the teaching of the graduate transport phenomena course. We have illustrated these numerical codes by

Table 4 Values at the Collocation Points of the Solution of the Transient Poiseuille Flow Problem at $\tau = 0.1359$

j	y_j	u_j^a	u_j^b
0	1.0000	0	−0.0000
1	0.9938	0.0084	0.0084
2	0.9755	0.0326	0.0326
3	0.9455	0.0706	0.0706
4	0.9045	0.1188	0.1188
5	0.8536	0.1732	0.1731
6	0.7939	0.2295	0.2294
7	0.7270	0.2839	0.2838
8	0.6545	0.3335	0.3333
9	0.5782	0.3764	0.3762
10	0.5000	0.4117	0.4114
11	0.4218	0.4394	0.4390
12	0.3455	0.4602	0.4598
13	0.2730	0.4751	0.4747
14	0.2061	0.4852	0.4847
15	0.1464	0.4916	0.4911
16	0.0955	0.4952	0.4947
17	0.0545	0.4970	0.4965
18	0.0245	0.4977	0.4972
19	0.0062	0.4979	0.4973
20	0	0.4979	0.4973

[a]Chebyshev collocation method.
[b]Separation of variables method.

Table 5 Values at the Collocation Points of the Solution of the Transient Couette Flow Problem at $t = 0.1255$ for $v = 0.1$

j	y_j	u_j^a	u_j^b
0	1.0000	0	−0.0000
1	0.9938	0.0000	0.0000
2	0.9755	0.0000	0.0000
3	0.9455	0.0000	0.0000
4	0.9045	0.0000	0.0000
5	0.8536	0.0000	0.0000
6	0.7939	0.0000	0.0000
7	0.7270	0.0000	0.0000
8	0.6545	0.0000	0.0000
9	0.5782	0.0003	0.0003
10	0.5000	0.0016	0.0016
11	0.4218	0.0079	0.0078
12	0.3455	0.0295	0.0292
13	0.2730	0.0854	0.0849
14	0.2061	0.1940	0.1933
15	0.1464	0.3561	0.3554
16	0.0955	0.5474	0.5467
17	0.0545	0.7313	0.7309
18	0.0245	0.8775	0.8773
19	0.0062	0.9691	0.9690
20	0	1.0000	1.0000

[a]Chebyshev collocation.
[b]Separation of variables.

presenting details of some of the highly nonlinear problems that were selected as illustrative examples.

In the recent past, the teaching of transport phenomena revolved around two issues: setting up mathematical models and associated initial and boundary conditions, and derivation of analytical solutions mostly for asymptotic cases of the mathematical models. Nowadays, the integration of powerful and rather user-friendly numerical codes, such as Matlab and Mathematica, in chemical engineering education is worthwhile. This integration of such codes allows the instructor and the student to broaden their horizons by attempting to tackle nonlinear problems typical of real-life engineering problems with relative ease.

Needless to say, educators should exhibit considerable flexibility in their curriculum and need to move rapidly to keep up with the rapidly changing computational environment. The work described here is presented in that spirit.

Finally, all the codes are available upon request from the corresponding author.

APPENDIX A

Advanced Transport Phenomena I (CHE 501)

First Semester 2013–2014 (Term 131)

Objective: Continuum theory of momentum, energy and mass transfer. Viscous behavior of fluids. Molecular transport mechanisms. General property balance. Laminar and Turbulent flow. Convective transport. Momentum, heat and mass applications of transport phenomena.

Prerequisites: Graduate Standing

Outcomes:

Understand the similarities between the different types of transport phenomena

Apply knowledge of advanced mathematics, science, and engineering principles in solving chemical engineering problems.

Formulate transport phenomena problems and set boundary conditions for solving differential equations.

Conduct independent research projects.

Communicate effectively orally and in writing.

Use Matlab and Mathematica to solve problems related to momentum, heat and mass transfer.

Textbook: Transport Phenomena, by Bird, Steward and Lightfoot, 2nd Edition, Wiley, 2007.

Topics:	Chapters in BSL
1 Introduction to transport phenomena Introduction to molecular transport	Chapters 0, 1, 9, 17 and Appendix A of BSL
2. Velocity distribution in laminar flow	Chapters 2, 10, 18 of BSL
3. Development of mass, momentum and energy conservation equations—Navier–Stokes equations and inviscid flow	Chapters 3, 11, and 19 of BSL
4. Velocity distribution with more than one independent variable.	Chapter 4 of BSL

Grading System:

HW Assignments	10%
Mid Term	30%
Project	20%
Final Exam	40%

APPENDIX B

```
DerivativeMatrix[Np_] := Module[{d, i, j, k, y, dM},
  d[0, 0] = (2 Np^2 + 1)/6 // N; d[Np, Np] = -d[0, 0];
  d[0, Np] = (-1)^Np/2 // N; d[Np, 0] = -d[0, Np];
  y[i_] := Cos[i π/Np] // N;
  d[i_, i_] := If[ i ≠ 0 && i ≠ Np, -y[i]/(2 (1 - y[i]^2))] // N;
  d[j_, k_] := If[j ≠ k && k ≠ 0 && j ≠ 0 && k ≠ Np && j ≠ Np, (-1)^(j+k)/(y[j] - y[k])] // N;
  d[j_, 0] := If[ j ≠ Np && j ≠ 0 , (-1)^j/(2 (y[j] - y[0]))] // N;
  d[0, k_] := If[ k ≠ Np && k ≠ 0 , 2 (-1)^k/(y[0] - y[k])] // N;
  d[j_, Np] := If[ j ≠ Np && j ≠ 0 , (-1)^(j+Np)/(2 (y[j] - y[Np]))] // N;
  d[Np, k_] := If[k ≠ Np && k ≠ 0 , 2 (-1)^(Np+k)/(y[Np] - y[k])] // N;
dM = Table[d[i, j], {i, 0, Np}, {j, 0, Np}]]
```

The implementation can be tested for $N_p = 5$ through comparison with the results given in Ref. [16]:

$$D = \text{DerivativeMatrix}[5]$$

$$\begin{pmatrix} 8.5 & -10.47 & 2.894 & -1.528 & 1.106 & -500.\times 10^{-3} \\ 2.618 & -1.171 & -2. & 894.4\times 10^{-3} & -618.\times 10^{-3} & 276.4\times 10^{-3} \\ -723.6\times 10^{-3} & 2. & -170.8\times 10^{-3} & -1.618 & 894.4\times 10^{-3} & -382.\times 10^{-3} \\ 382.\times 10^{-3} & -894.4\times 10^{-3} & 1.618 & 170.8\times 10^{-3} & -2. & 723.6\times 10^{-3} \\ -276.4\times 10^{-3} & 618.\times 10^{-3} & -894.4\times 10^{-3} & 2. & 1.171 & -2.618 \\ 500.\times 10^{-3} & -1.106 & 1.528 & -2.894 & 10.47 & -8.5 \end{pmatrix}$$

$$D^2 = \text{DerivativeMatrix}[5] \bullet \text{DerivativeMatrix}[5]$$

$$\begin{pmatrix} 41.6 & -68.36 & 40.83 & -23.64 & 17.57 & -8. \\ 21.29 & -31.53 & 12.68 & -3.694 & 2.211 & -952.8\times 10^{-3} \\ -1.847 & 7.317 & -10.07 & 5.789 & -1.906 & 714.1\times 10^{-3} \\ 714.1\times 10^{-3} & -1.906 & 5.789 & -10.07 & 7.317 & -1.847 \\ -952.8\times 10^{-3} & 2.211 & -3.694 & 12.68 & -31.53 & 21.29 \\ -8. & 17.57 & -23.64 & 40.83 & -68.36 & 41.6 \end{pmatrix}$$

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