Appendix A

The aim of this additional material is on one hand, introducing the algebraic system used to construct all the non-arbitrary graphics of this paper, and on another hand, presenting a detailed solution process, step by step.

Consider the following illustrative problem noted by Kuno and Seader[39].

Given the nonlinear system of two equations

$$F_1(x_1,x_2) = 2x_1^3 + 2x_1x_2 - 21x_1 + x_2^2 - 7 \tag{A1}$$

$$F_1(x_1,x_2) = x_1^2 + 2x_1x_2 + 2x_2^3 + 13x_2 - 11 \tag{A2}$$

Determine one zero of the system using the Fixed-point homotopy form and horizontal predictors.

Horizontal predictors are simple increments of the homotopic parameter to obtain the next point of the homotopic curve. Thus, the solution is:

1. Defining an arbitrary initial guess

   $x_1^0 = 2.0$ and $x_2^0 = 2.0$

2. Thus, the simpler system ($E(x)$) for Fixed-point homotopy form is given by Equation 4, which is

   $E(x) = x - x^0$

   Replacing the initial guess defined in step 1 in the two equations that forms the vectorial equation of step 2 (Equation 4 of the paper).

$$E_1(x_1, x_2) = x_1 - 2 \tag{A3}$$

$$E_2(x_1, x_2) = x_2 - 2 \tag{A4}$$

3. From the observations made for Equation 2, the method requires that the homotopic variable t is set to 0 for the values defined for the initial guess. Substituting $t = 0$ in this equation yields

$$H(x,t) = (0)F(x) + (1-0)E(x) = E(x) = 0 \tag{A5}$$

Which can be restated as follows:

$$H_1(t, x_1, x_2) = x_1 - 2 = 0 \tag{A6}$$

$$H_2(t, x_1, x_2) = x_2 - 2 = 0 \tag{A7}$$

The initial guess clearly satisfies to the homotopic system at $t = 0$

4. So, according with the homotopic paradigm $E(x)$ can be deformed within the homotopic mapping function by simply augmenting the homotopic parameter.

Proposing $\Delta t = 0.1$

A new system is defined for $t = t + \Delta t = 0 + 0.1 = 0.1$. Eqution 2 is now transformed into

$$H(x,t) = (0.1)F(x) + (1-0.1)E(x) = E(x) = 0 \tag{A8}$$

In other words, for the two equations

$$H_1(t, x_1, x_2) = (0.1)(2x_1^3 + 2x_1x_2 - 21x_1 + x_2^2 - 7) + 0.9(x_1 - 2) = 0 \tag{A9}$$

$$H_2(t,x_1,x_2)=(0.1)(x_1^2+2x_1x_2+2x_2^3+13x_2-11)+0.9(x_2-2)=0 \tag{A10}$$

This expression constitutes the second point of the homotopic parameter to be calculated. Again, according with the homotopic paradigm, Equations A9 and A10 form a system that topologically approximates the previous system (formed by Equations A6 and A7). Thus, the solution of the first one system (Equations A6 and A7) can be used as the initial guess to solve the second one by a local method, such as the Newton method, which can be consulted in almost any numerical methods textbook. The system was solved using a computer code for the classical Newton method written in Fortran 90®; the obtained results and technical data are shown in the first row of Table A1.

With the values for x_1, x_2 obtained by the Newton method for the specified value of t, another itration can be computed.

5. Again, to calculate the next step, the value of t has to be modified $t=t+\Delta t=0.1+0.1=0.2$, which defines the new system, in vectorial form

$$H(x,t)=(0.2)F(x)+(1-0.2)E(x)=E(x)=0 \tag{A11}$$

In other words, the two homotopic equations are

$$H_1(t,x_1,x_2)=(0.2)(2x_1^3+2x_1x_2-21x_1+x_2^2-7)+0.8(x_1-2)=0 \tag{A12}$$

$$H_2(t,x_1,x_2)=(0.2)(x_1^2+2x_1x_2+2x_2^3+13x_2-11)+0.8(x_2-2)=0 \tag{A13}$$

The system described by A11 topologically approximates the system described by A8. Thus, the solution of A8 will likely converge to the solution of A11. The results in the second row of Table A1 were generated by solving the two equations, A12 and A13, in the same way that system A8 was solved.

With the values for x_1, x_2 obtained by the Newton method for the specified value of t, another itration can be computed.

6. Repeating the process; $t = t + \Delta t = 0.2 + 0.1 = 0.3$, the vectorial form of the homotopic system is

   $$H(x,t) = (0.3)F(x) + (1-0.3)E(x) = E(x) = 0 \tag{A14}$$

   In other words, the two homotopic equations are

   $$H_1(t, x_1, x_2) = (0.3)(2x_1^3 + 2x_1x_2 - 21x_1 + x_2^2 - 7) + 0.7(x_1 - 2) = 0 \tag{A15}$$

   $$H_2(t, x_1, x_2) = (0.3)(x_1^2 + 2x_1x_2 + 2x_2^3 + 13x_2 - 11) + 0.7(x_2 - 2) = 0 \tag{A16}$$

   The system A14 topologically approximates the system A11. Thus, the solution of A11 will likely converge to the solution of A14. The results in the third row of Table A3 were generated by solving the two equations, A15 and A16, in the same way that system A8 was solved.

7. The process presented above is repeated until t reaches a value of 1, a complete list of the results obtained by the complete numerical process is shown in Table A1

8. A graph of the homotopic variables (t, x_1, x_2) that form the homotopic path is shown in Fig. A1.

9. The current example have been extensively solved in the literature, proving that there are more than one root (actually nine zeros are known)[39]. We use this example

with Fixed-point homotopy and the appropriate initial guess to get an only one root in the opened homotopic path section that is connected to the initial guess, only to illustrate more clearly the essence of homotopic solution processes. Using a the hyperspherical path tracking methodology[68] with Newton homotopy and the initial guess $x^0 = [1,1]^t$, the nine known solution vectors can be obtained (Table A2). The homotopic path in N+1 dimensional space (3-D for this case) is shown in Fig. A2, and 2-D and 3-D representations of the nine roots are depicted in Fig. A3.

Figure Captions

Fig. A1. Homotopic path for the two partial derivatives of Himmelblau function (Example of Appendix A) with an initial guess $x_1 = 2, x_2 = 2$ and Fixed-point homotopy.

Fig. A2. Homotopic path for the two partial derivatives of Himmelblau function (Example of Appendix A) with an initial guess $x_1 = 1, x_2 = 1$ and Newton homotopy.

Fig. A3. Geometrical localization of the nine roots for the two partial derivatives of Himmelblau function (Example of Appendix A the curves and surfaces for f_1 are shown in red and green for f_2). (a) 3-D representation. (b) 2-D representation. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)

Table 1. Applications of homotopic methods in chemical engineering

Application	Contribution	Reference
Fluid mechanics • Elliptic porous slider • Compression of a fluid between two plates • Deceleration of rotating disks for viscous fluids • Flow in a porous channel of a rotational system • Optimization (nonlinear complementary problems)	Application of the Yorke algorithm on FORTRAN a known code named HOMPACK 77	52
Absorption Columns	Homotopic first tracking algorithms.	103
Different configurations in distillation columns interconnected.	First applications of the differential tracking method with respect to the arc length of the homotopic path.	56
Reaction in a catalytic particle, diffusion problem with auto catalysis and hypersonic flow.	Implementation of tracking algorithms with a focus on the management of branches.	21
Engineering flowcharts	Affine homotopy to prevent cyclic paths	22
Resolution of equations diffusion type in semi-conductors	Combination of finite element method with tracking arc length parameterization of the homotopic path	104

Table 1. Continuation

Application	Details	Reference
Numerical solution of mass balances for continuous stirred reactors with radical intermediates.	Application of transformation methods for selecting the initial guesses used in Fixed-point homotopy	105
Calculating azeotropes in more than one phase for multicomponent mixtures.	Application of methods of detection of bifurcations	106
Analysis of reactive multiphase systems	Application tracking algorithm with forks and branches handling complex homotopy path.	107
Solution of mathematical models (Partial Differential Equations) steady state.	Solution of systems resulting from the discretization of differential equations.	108
A solution of reduced model for controlling an activated sludge process.	Application of homotopic methods in biological reacting systems	109
Parameter estimation for elliptic PDE	Combination of monitoring homotopic to the method of regularization Tikonov	110
Simulated distillation columns with calculation of the equilibrium curves for ternary mixtures.	Application of penalty functions for parameter homotopy of homotopies defined.	58

Table A1. Numerical results for the complete homotopic path tracking of the problem defined in appendix A1 using: 10 equidistant steps, a tolerance value of $1x10^{-8}$, and an increment value for numerical derivation of $1x10^{-6}$

Step	t	x_1	x_2	Iterations of Newton method
0	0	2	2	-
1	0.1	2.765338	2.086213	7
2	0.2	2.883727	2.053658	5
3	0.3	2.929434	2.035706	5
4	0.4	2.953682	2.024648	4
5	0.5	2.968720	2.017185	4
6	0.6	2.978962	2.011816	4
7	0.7	2.986388	2.007769	4
8	0.8	2.992021	2.004611	4
9	0.9	2.996440	2.002077	4
10	1.0	3.000000	2.000000	4

Table A2. The nine known solution vectors for the two partial derivatives of Himmelblau function (problem defined in appendix A1)

Vector	x_1	x_2	$f_1(x_{1,}x_2)$	$f_2(x_{1,}x_2)$
1	0.086677506	2.884254703	-5.85395×10^{-9}	8.80663×10^{-8}
2	-2.805118089	3.13131252	-7.48616×10^{-8}	5.38551×10^{-8}
3	-3.073025754	-0.08135304	-1.36472×10^{-7}	-7.02011×10^{-8}
4	-3.779310261	-3.283186001	-3.08118×10^{-7}	-3.36911×10^{-7}
5	-0.270844597	-0.923038526	7.56068×10^{-8}	-2.37774×10^{-7}
6	-0.127961343	-1.953714998	-1.1749×10^{-8}	-1.84292×10^{-7}
7	3.584428343	-1.848126546	8.36695×10^{-8}	-2.69014×10^{-7}
8	3.385154189	0.073851888	3.04466×10^{-7}	-1.48185×10^{-8}
9	2.999999998	2.000000022	1.27382×10^{-7}	3.48265×10^{-7}

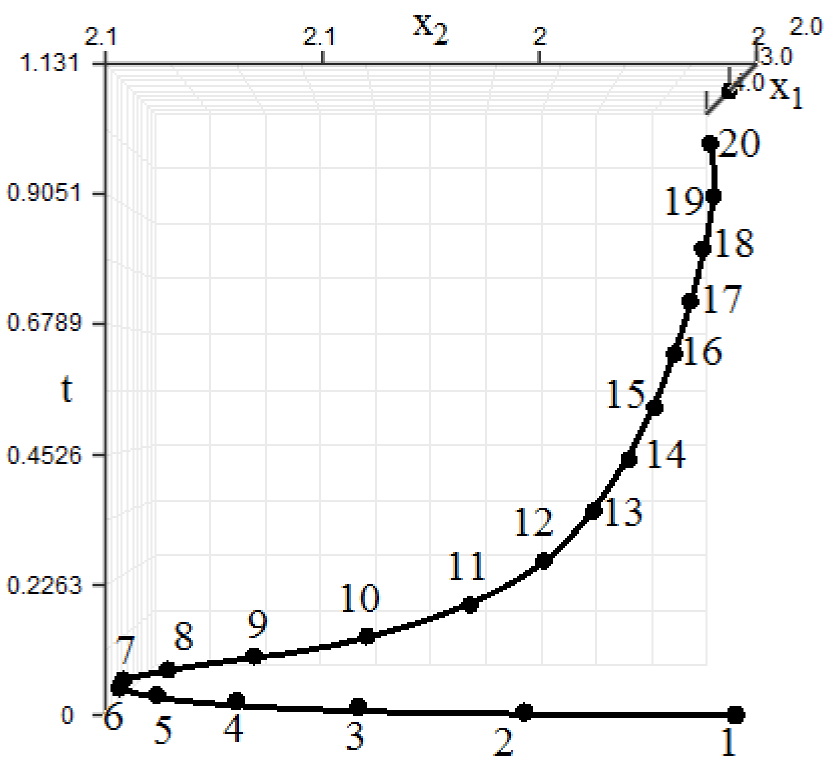


Fig. A1. Homotopic path for the two partial derivatives of Himmelblau function (Example of Appendix A) with an initial guess $x_1 = 2, x_2 = 2$ and Fixed-point homotopy.

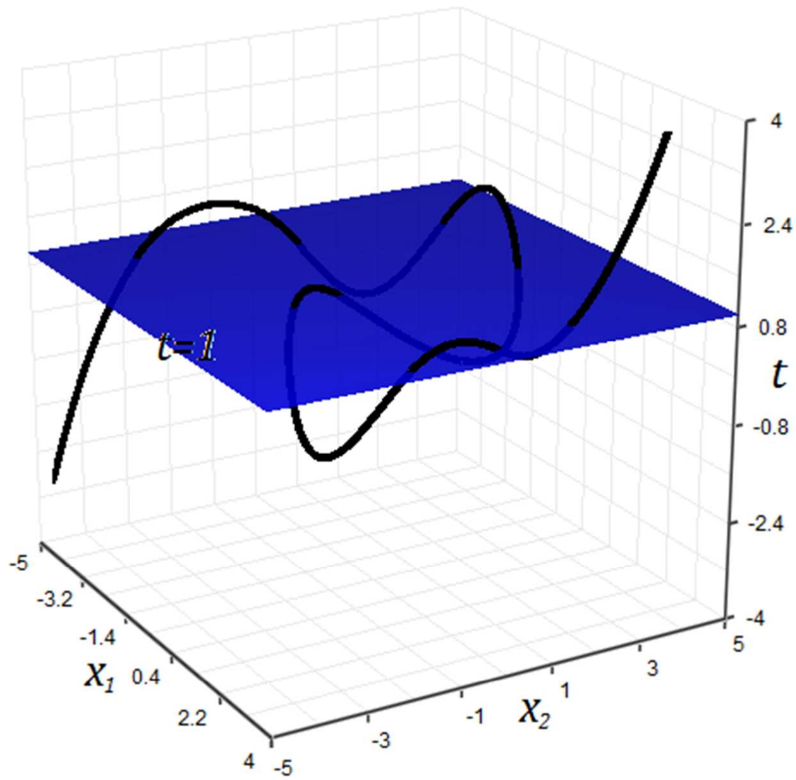
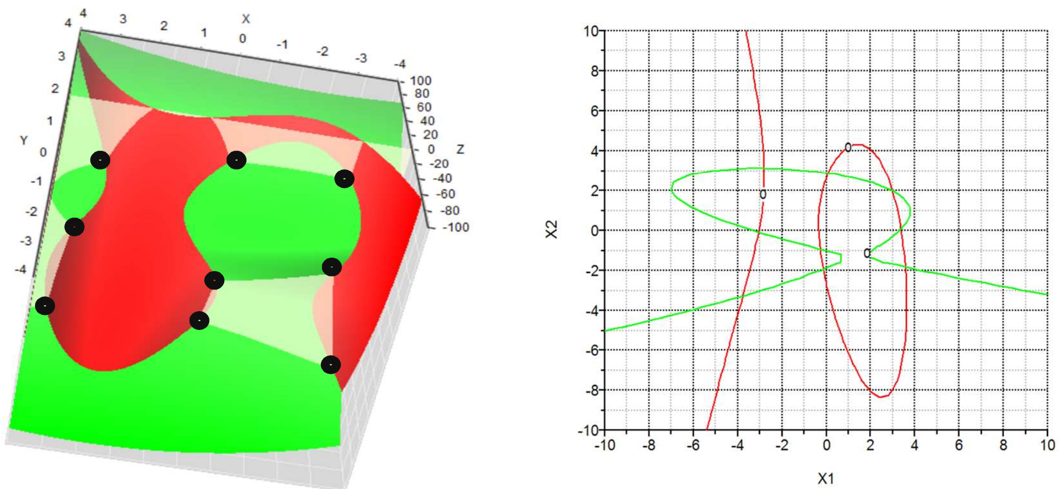


Fig. A2. Homotopic path for the two partial derivatives of Himmelblau function (Example of Appendix A) with an initial guess $x_1 = 1, x_2 = 1$ and Newton homotopy.



(a) (b)

Fig. A3. Geometrical localization of the nine roots for the two partial derivatives of Himmelblau function (Example of Appendix A; the curves and surfaces for f_1 are shown in red and green for f_2). (a) 3-D representation. (b) 2-D representation. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)