Blog Entry © Sunday, June 8, 2025, Chemical Reaction Kinetics by James Pate Williams, Jr.

We program solutions to two dimensionless activator-inhibitor mechanisms. The original equations were from a textbook [1]. For completeness we reproduce the first order non-linear ordinary differential equations, system 1:

$$\frac{du}{dt} = a - bu + \frac{u^2}{v}$$

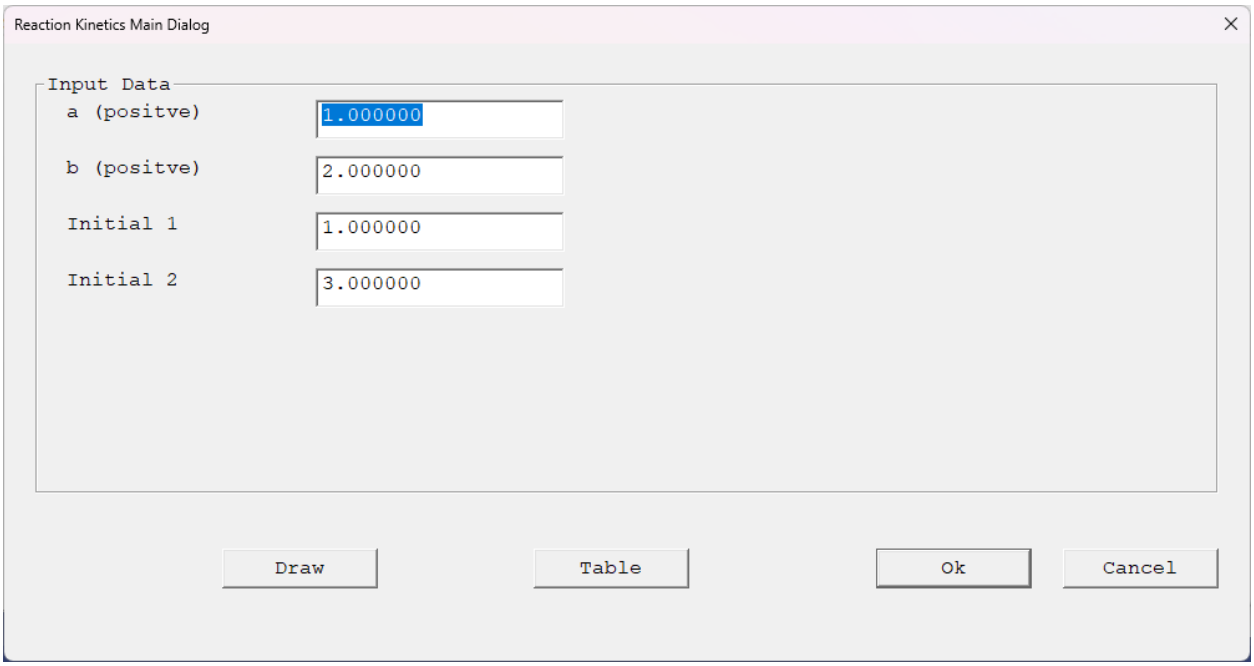
$$\frac{dv}{dt} = u^2 - v$$

Next, we have system 2:

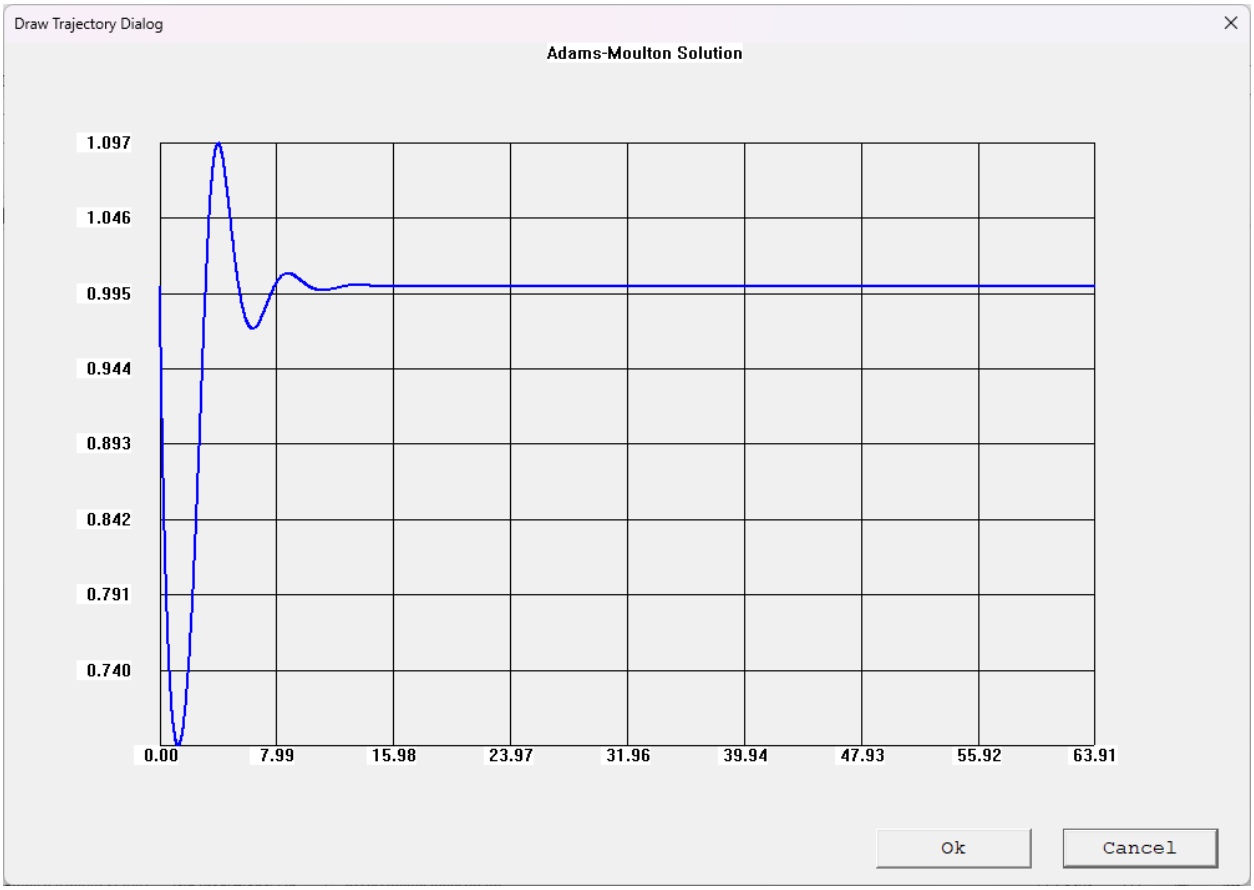
$$\frac{du}{dt} = a - u + u^2 v$$

$$\frac{dv}{dt} = b - u^2 v$$

The a and b are positive constants, and the initial values need to be positive. We used four algorithms to solve both previous systems: Adams-Moulton [2], Adams-Bashforth-Moulton [3], 5th order Runge-Kutta, and an algorithm from reference 3. The first screenshot is the main dialog's data entry window. We used the same constants and initial values throughout our experiments.



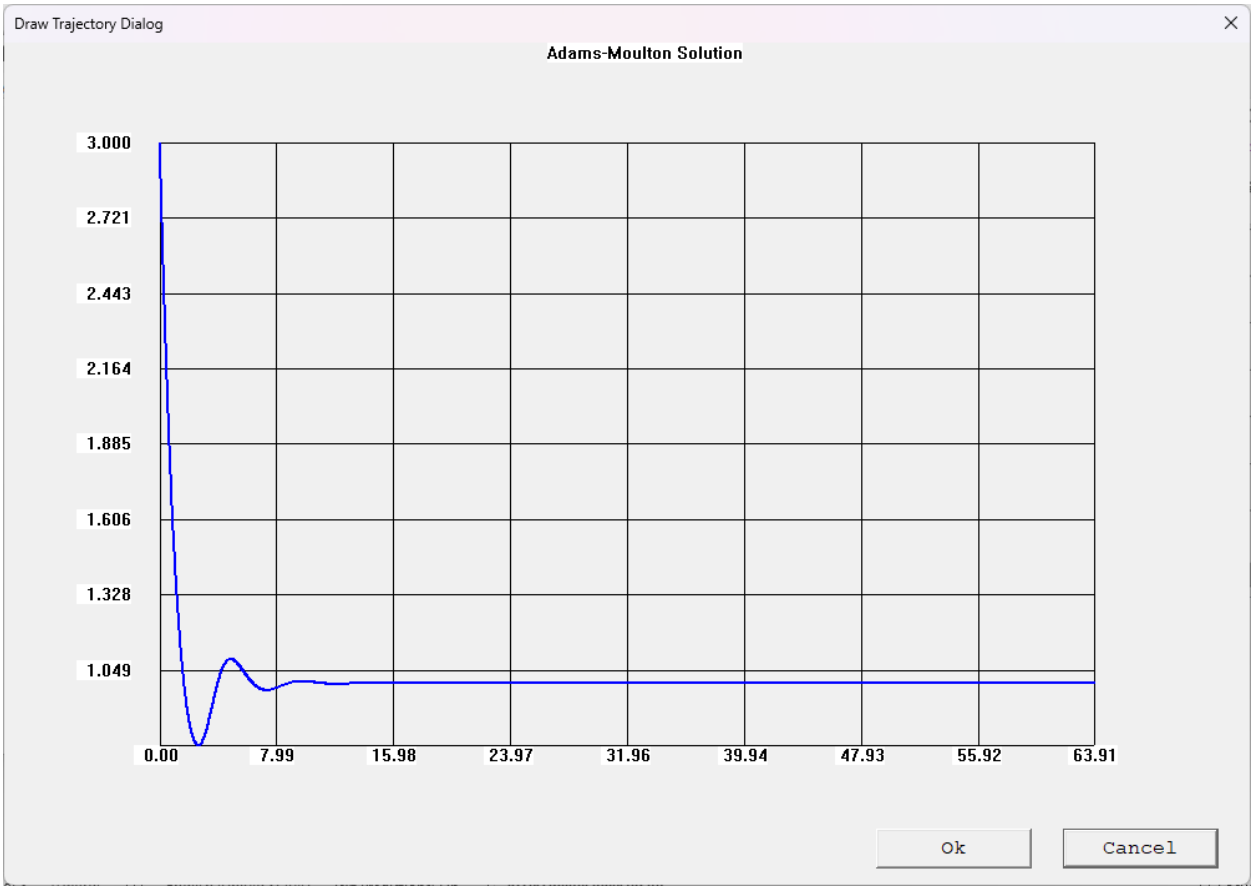
System 1 u(t):

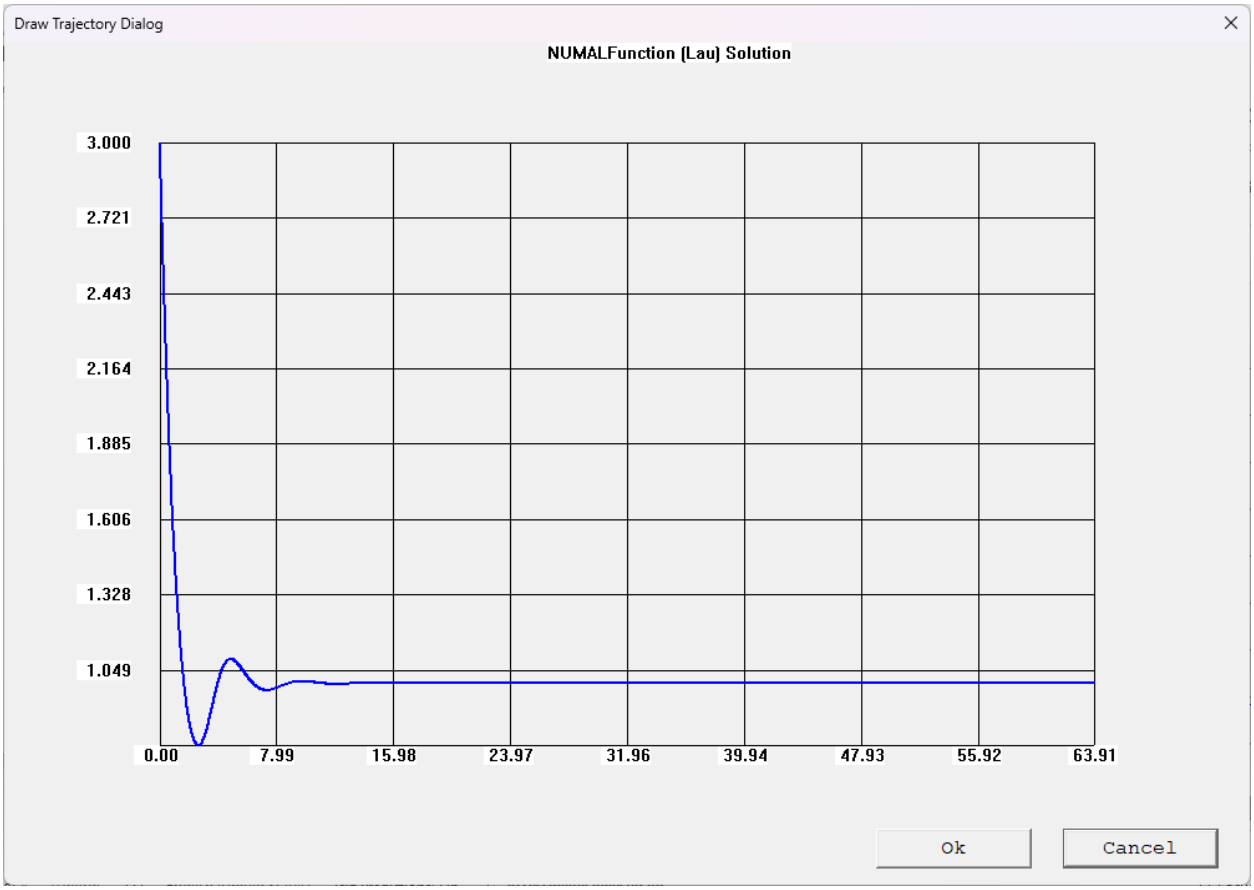

Draw Trajectory Dialog
Adams-Moulton Solution
1.097
1.046
0.995
0.944
0.893
0.842
0.791
0.740
0.00
7.99
15.98
23.97
31.96
39.94
47.93
55.92
63.91
Ok
Cancel

RKE function not displayed.

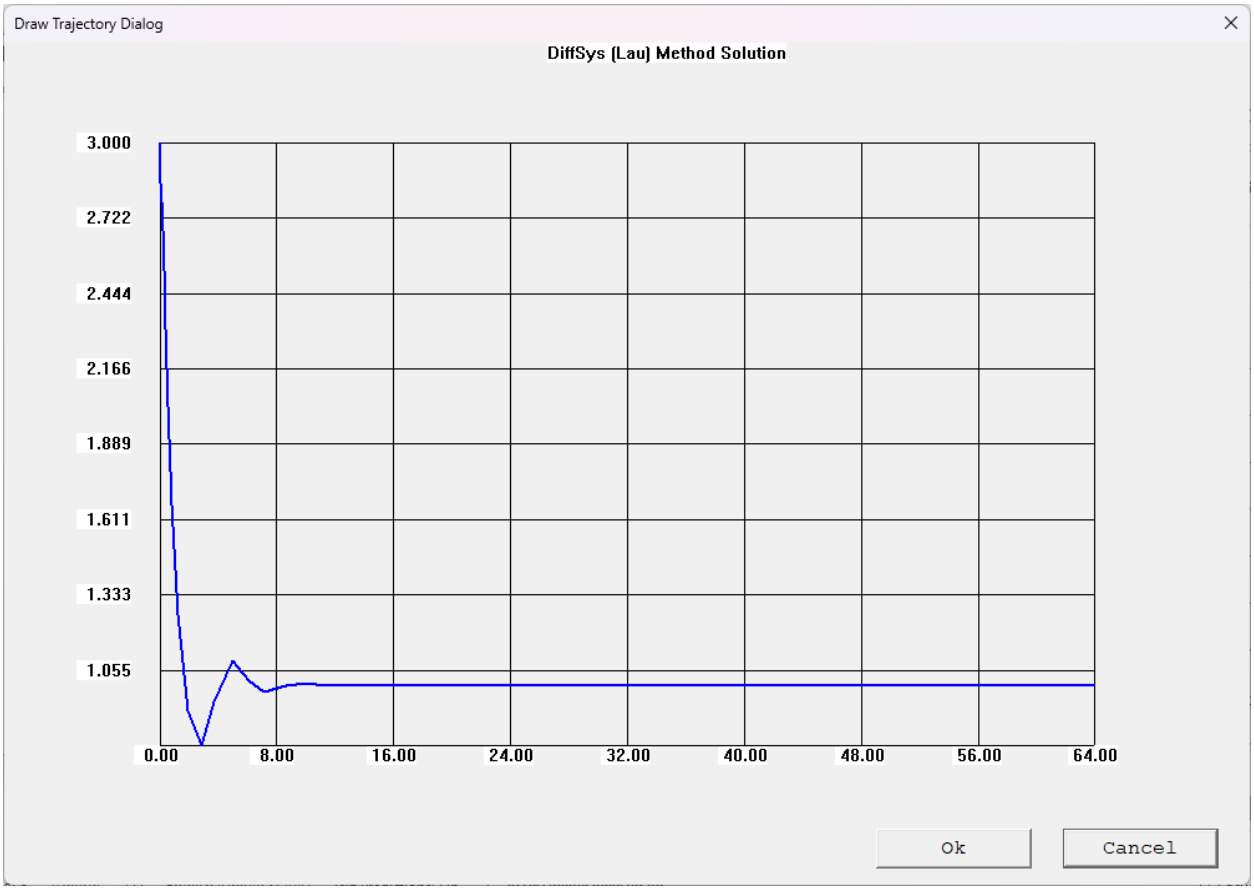

Draw Trajectory Dialog
DiffSys (Lau) Method Solution
1.084
1.034
0.985
0.936
0.887
0.837
0.788
0.739
0.00
8.00
16.00
24.00
32.00
40.00
48.00
56.00
64.00
Ok
Cancel

System 1 v(t):

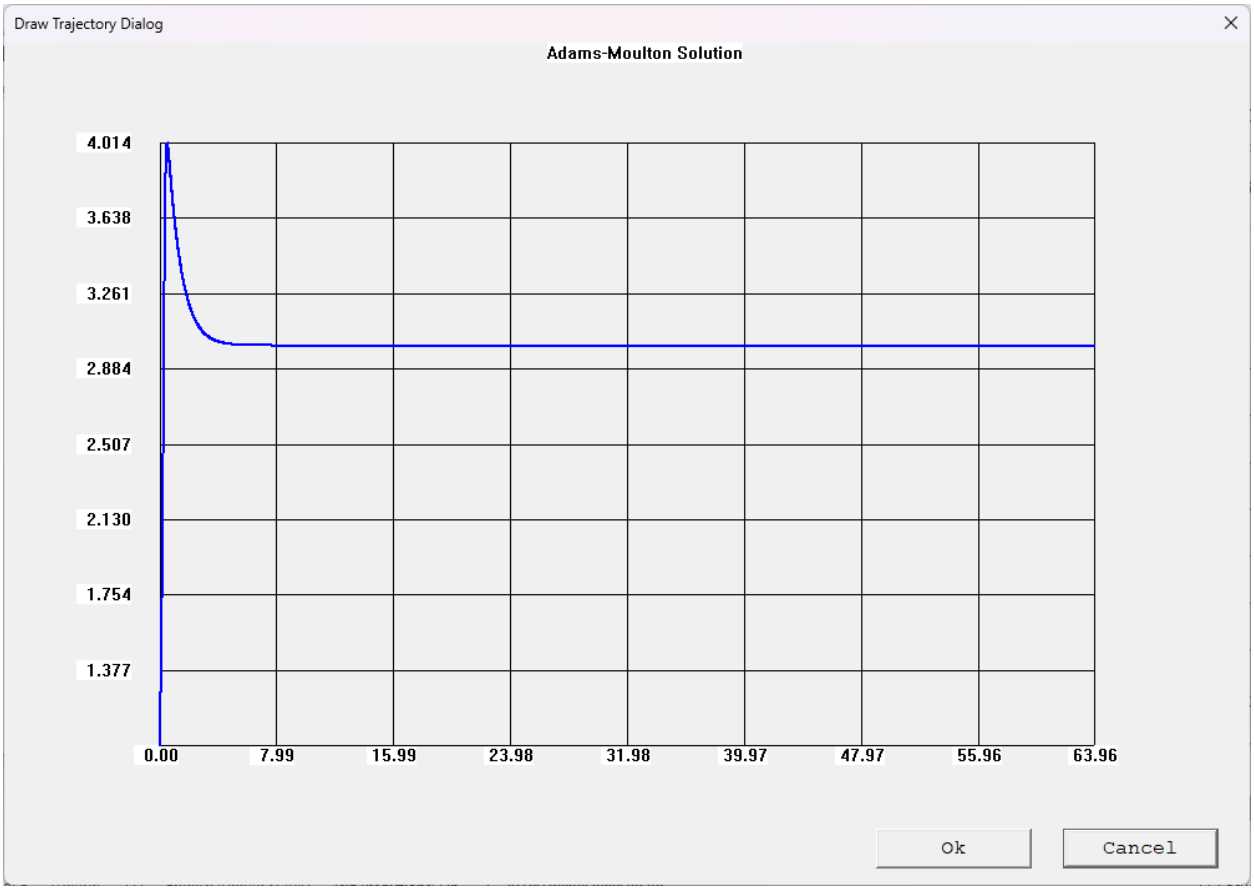

Draw Trajectory Dialog
Adams-Moulton Solution
3.000
2.721
2.443
2.164
1.885
1.606
1.328
1.049
0.00
7.99
15.98
23.97
31.96
39.94
47.93
55.92
63.91
Ok
Cancel

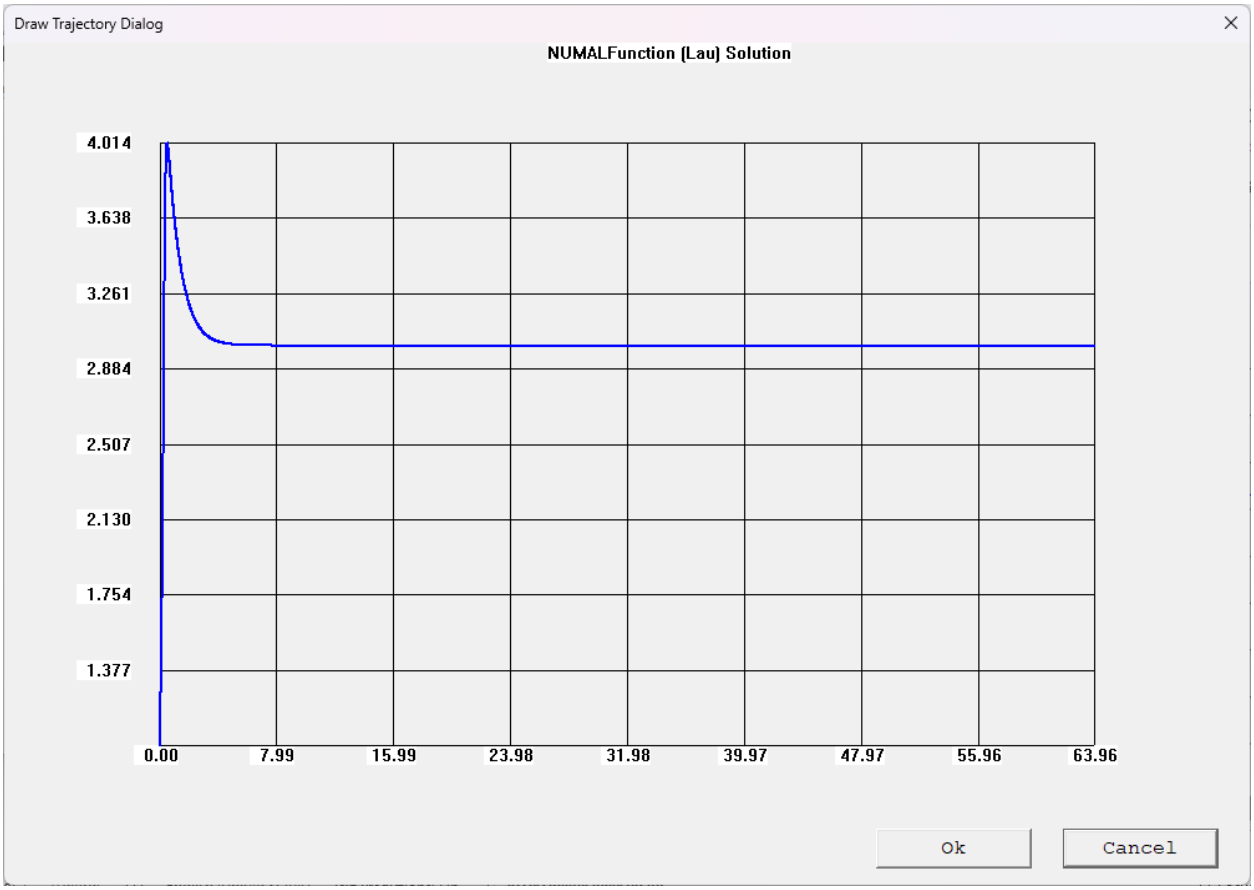


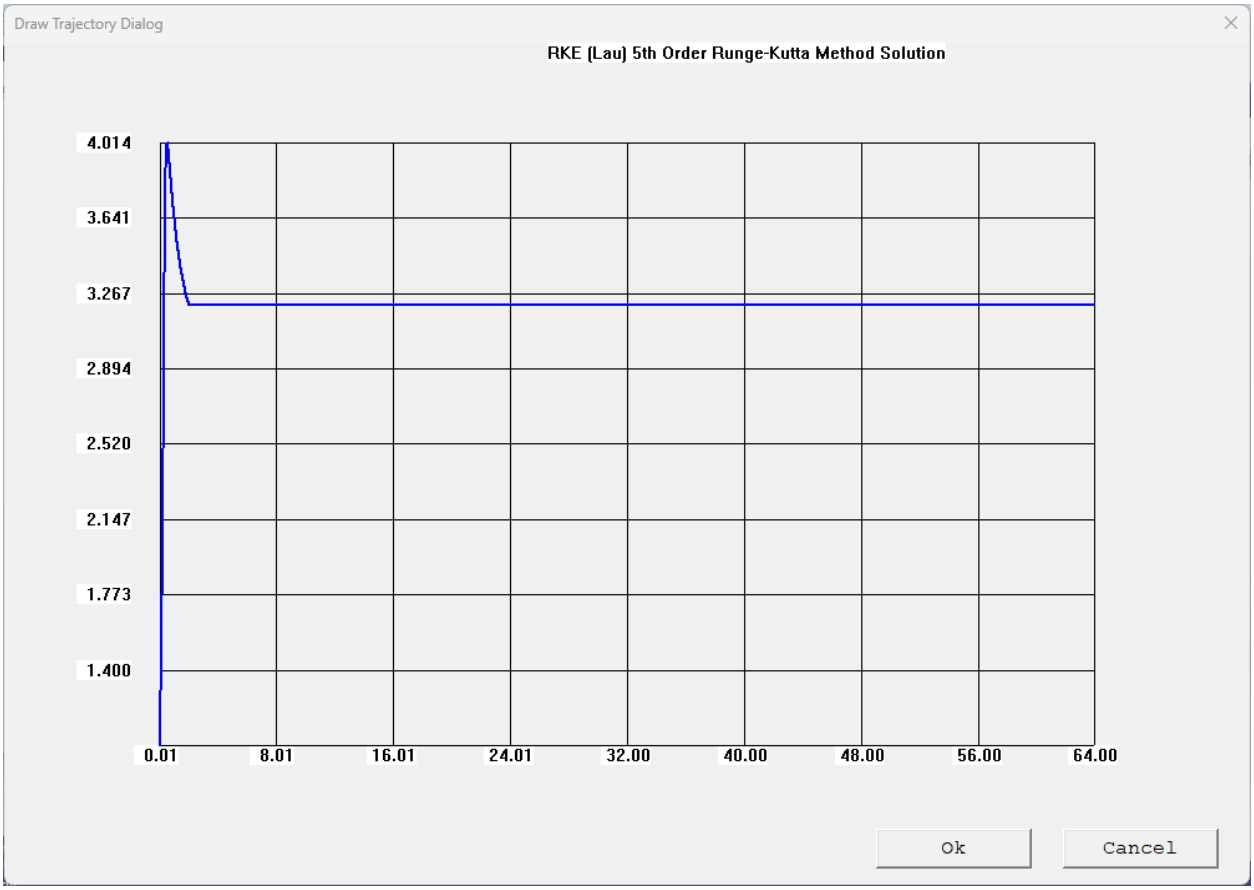
RKE function not displayed.

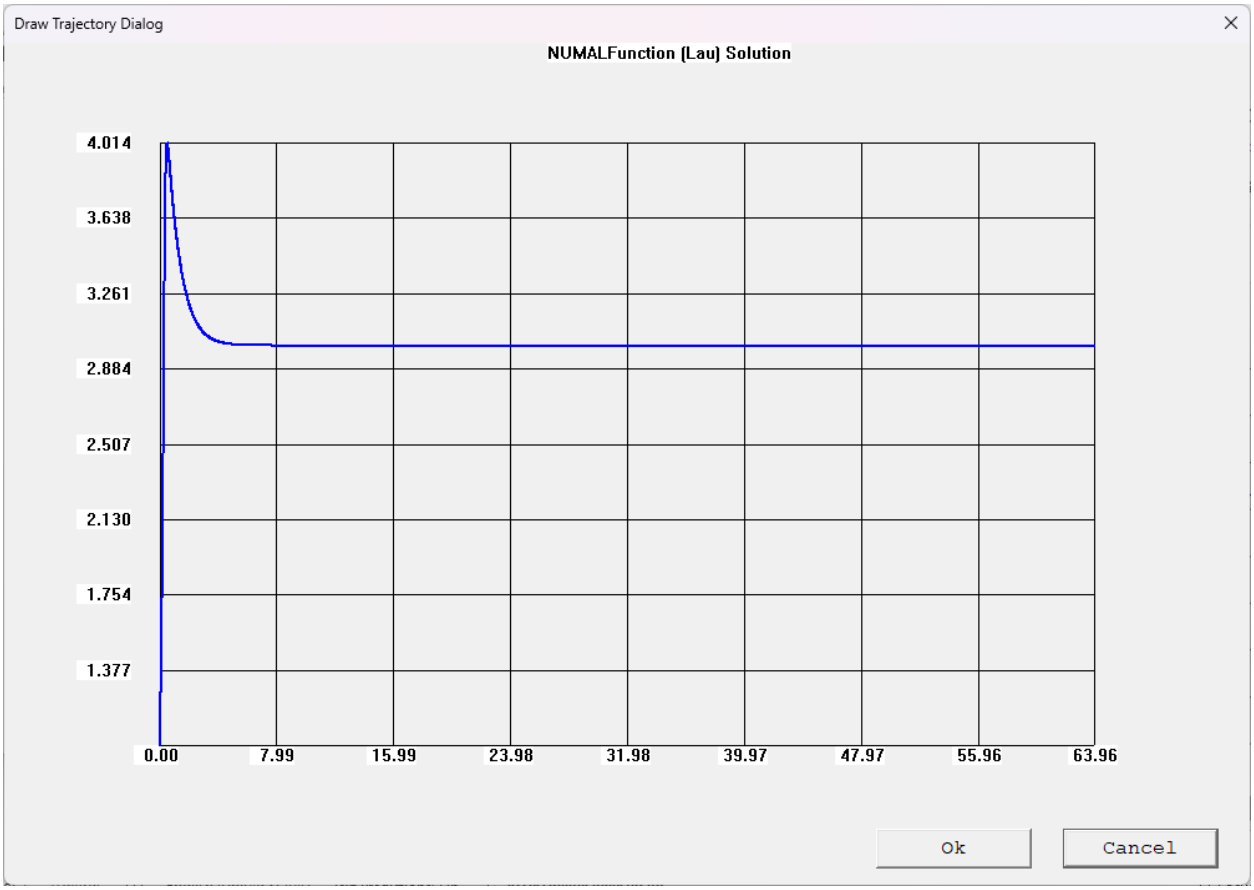

Draw Trajectory Dialog
DiffSys (Lau) Method Solution
3.000
2.722
2.444
2.166
1.889
1.611
1.333
1.055
0.00
8.00
16.00
24.00
32.00
40.00
48.00
56.00
64.00
Ok
Cancel

System 2 u(t):

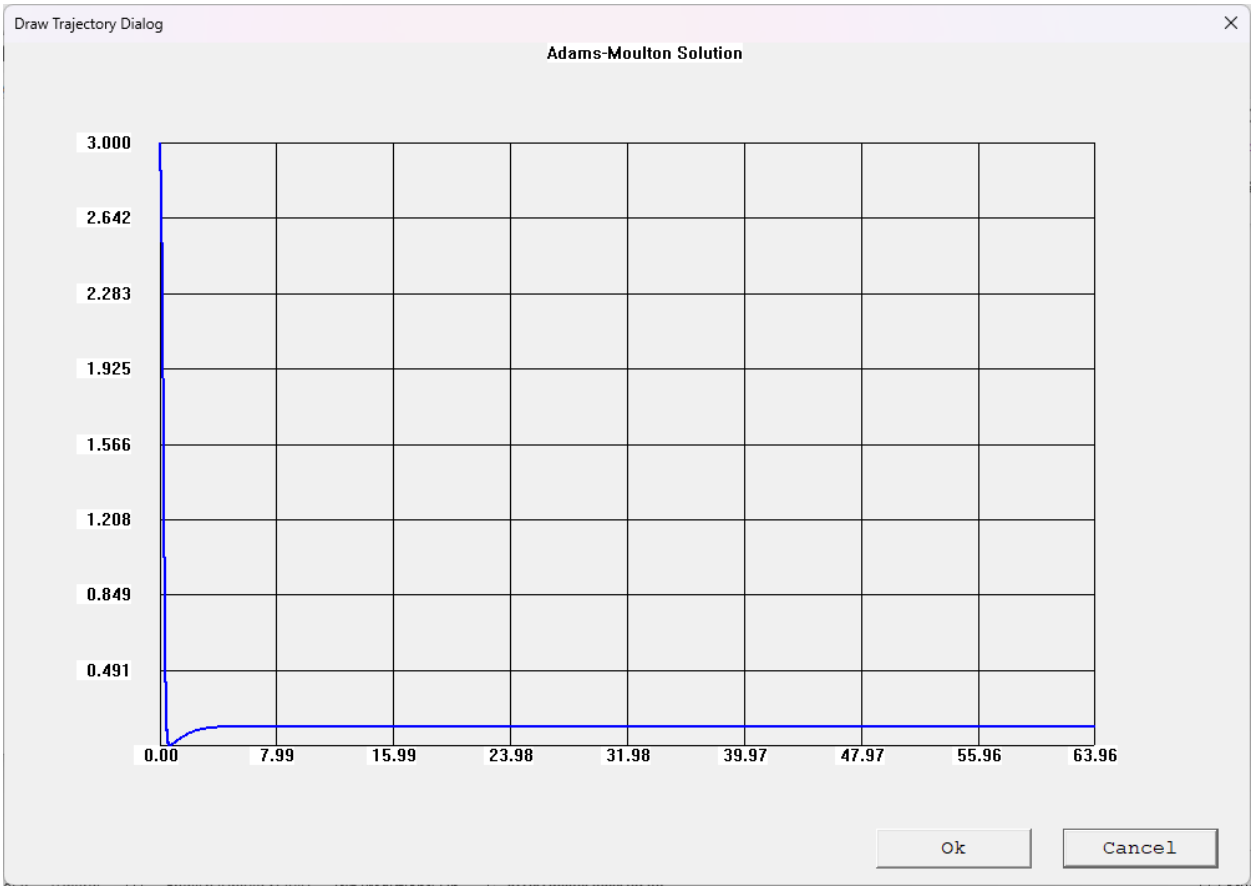

Draw Trajectory Dialog
Adams-Moulton Solution
4.014
3.638
3.261
2.884
2.507
2.130
1.754
1.377
0.00
7.99
15.99
23.98
31.98
39.97
47.97
55.96
63.96
Ok
Cancel

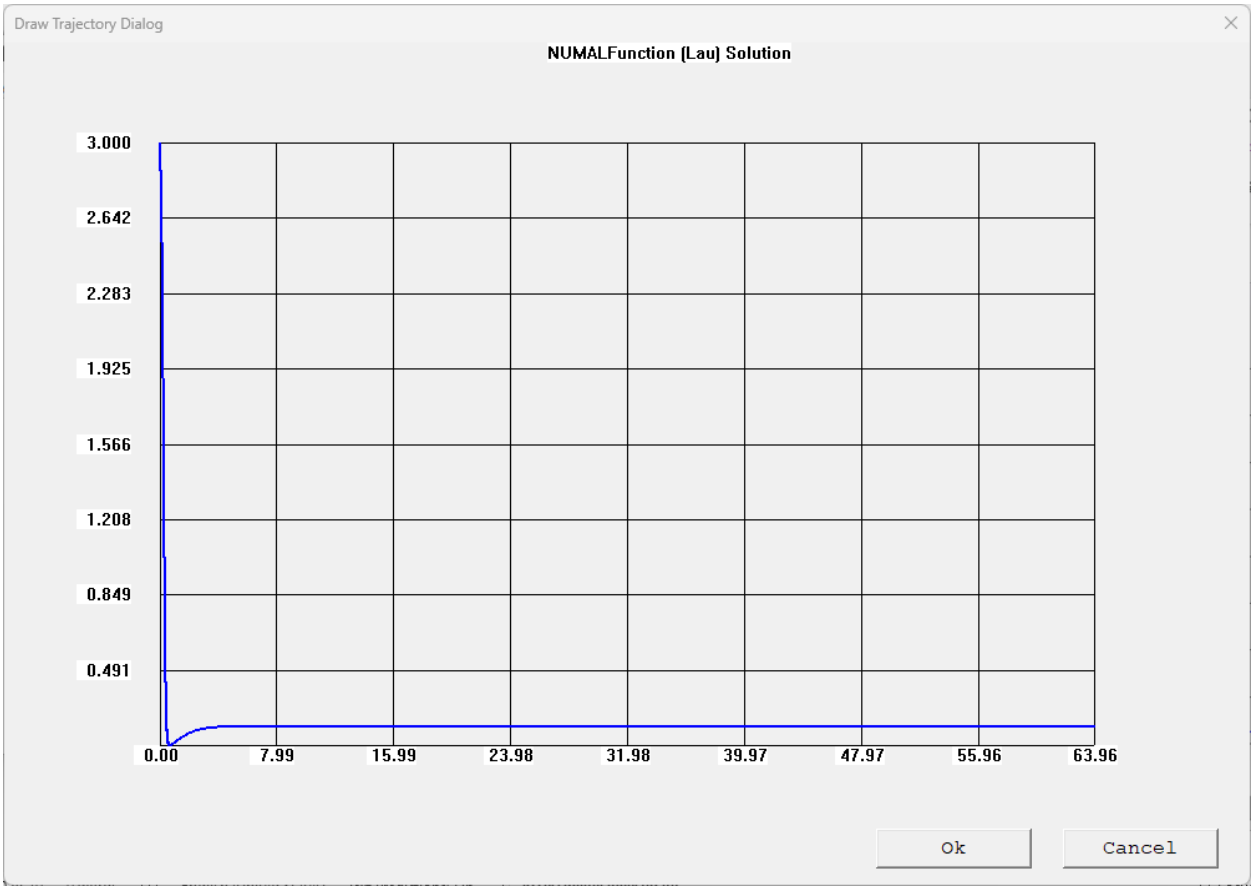

Draw Trajectory Dialog
NUMALFunction (Lau) Solution
4.014
3.638
3.261
2.884
2.507
2.130
1.754
1.377
0.00
7.99
15.99
23.98
31.98
39.97
47.97
55.96
63.96
Ok
Cancel

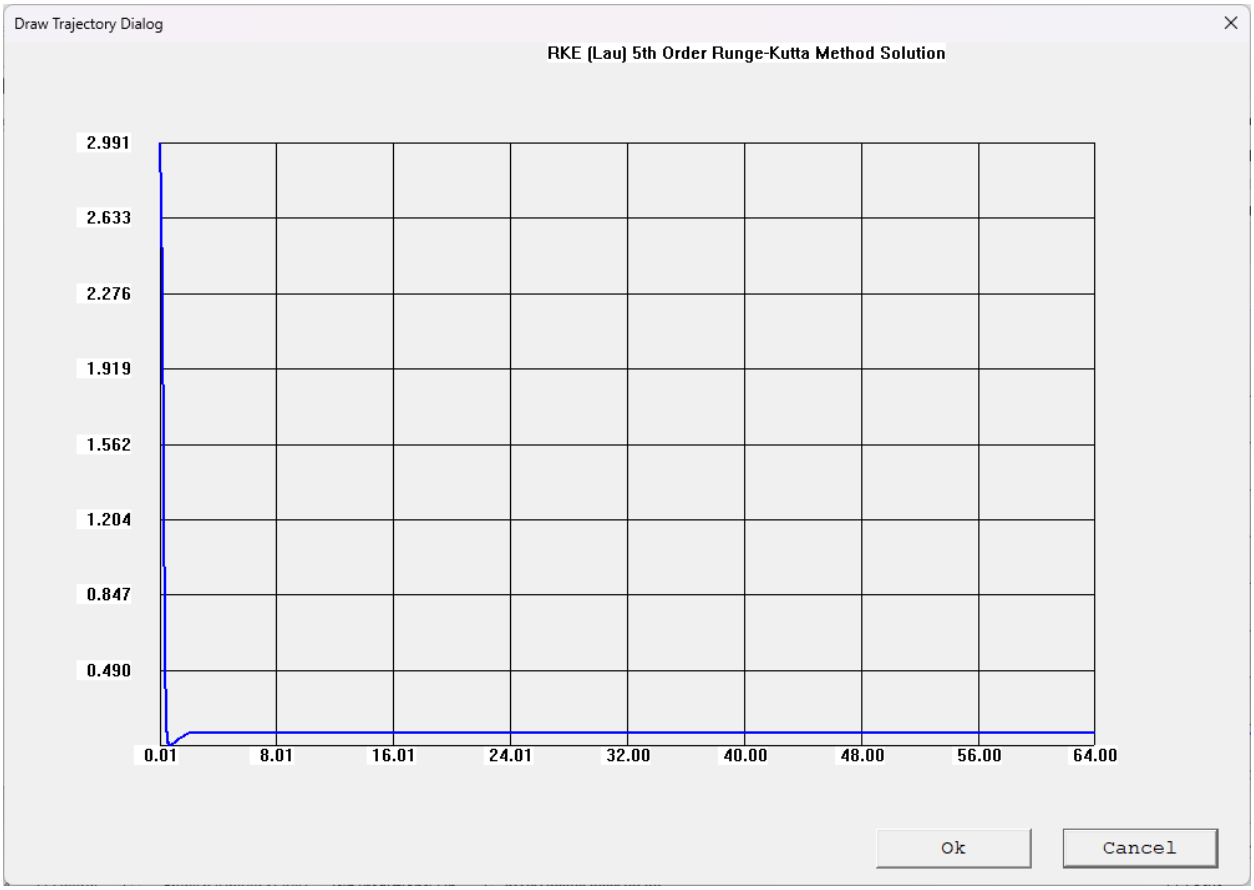

Draw Trajectory Dialog
RKE (Lau) 5th Order Runge-Kutta Method Solution
4.014
3.641
3.267
2.894
2.520
2.147
1.773
1.400
0.01
8.01
16.01
24.01
32.00
40.00
48.00
56.00
64.00
Ok
Cancel

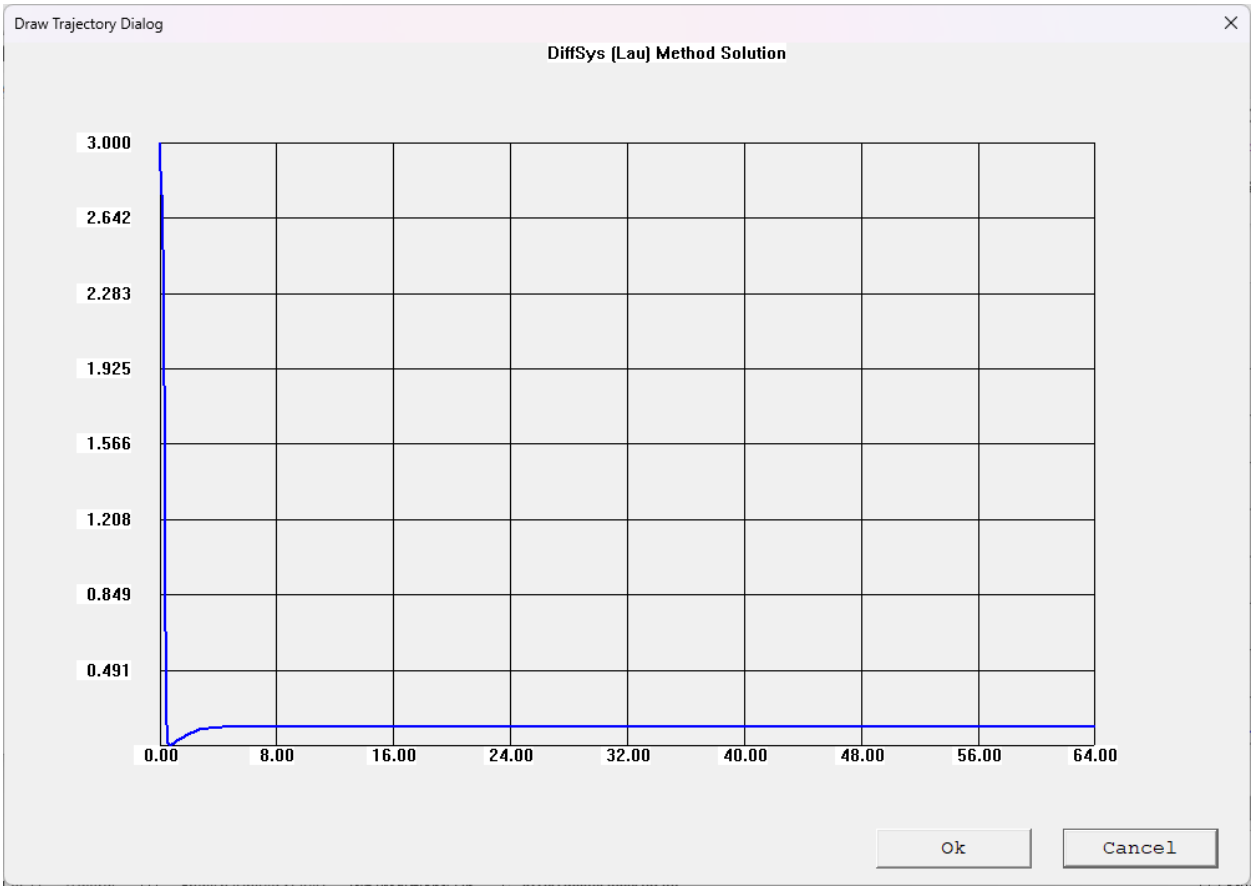

Draw Trajectory Dialog
NUMALFunction (Lau) Solution
4.014
3.638
3.261
2.884
2.507
2.130
1.754
1.377
0.00
7.99
15.99
23.98
31.98
39.97
47.97
55.96
63.96
Ok
Cancel

System 2 v(t):


Draw Trajectory Dialog
Adams-Moulton Solution
3.000
2.642
2.283
1.925
1.566
1.208
0.849
0.491
0.00
7.99
15.99
23.98
31.98
39.97
47.97
55.96
63.96
Ok
Cancel


Draw Trajectory Dialog
NUMALFunction (Lau) Solution
3.000
2.642
2.283
1.925
1.566
1.208
0.849
0.491
0.00
7.99
15.99
23.98
31.98
39.97
47.97
55.96
63.96
Ok
Cancel


Draw Trajectory Dialog
RKE (Lau) 5th Order Runge-Kutta Method Solution
2.991
2.633
2.276
1.919
1.562
1.204
0.847
0.490
0.01
8.01
16.01
24.01
32.00
40.00
48.00
56.00
64.00
Ok
Cancel



References

[1] J. D. Murray, "6. Reaction Kinetics," in *Mathmatical Biology I: An Introduction Third Edition*, New York, Springer , 2002, pp. 175-217.

[2] S. D. Conte and C. de Boor, "8.12 Systems of Differential Equations," in *Elementary Numerical Analysis An Algorithmic Approach Third Edition*, New York, McGraw-Hill Book Company, 1980, pp. 398-401.

[3] H. T. Lau, "Chapter 5: Analytic Problems," in *A Numerical Library in C for Scientists and Engineers*, Boca Raton, CRC Press, 1995, pp. 365-367.