Implicit Trapezoidal with Newton Rapshon

For solving moderately stiff nonlinear differential equations.

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1 Introduction

An ODE is ”stiff” when the rate of change of the solution lies within a wide range, from very slow to very fast. For explicit and constant step size methods like forward Euler, stiffness restricts selection of the step size as it should account for the fastest rate, and thereby increasing computational time and may also result in accumulation of errors. Implicit methods on the other hand are suitable for such problems.

1.1 Stiffness

Consider the equation (1) whose solution is equation (2).

$$y' = \lambda(-y + sinx) : y(0) = 0 \tag{1}$$

$$y(x) = C\exp^{-\lambda x} + \frac{\lambda^2}{1+\lambda^2}sinx - \frac{\lambda}{1+\lambda^2}cosx \tag{2}$$

For the initial condition $y = 0$ at $x = 0$, the constant C can easily be calculated to be $C = \frac{\lambda}{1+\lambda^2}$. For large values of λ we see that the solution grows exponentially when $x < 0$ while the exponential part decays for $x > 0$ and the solution $sin(x)$ is dominant. This uneven rate of change in solution causes stiffness.

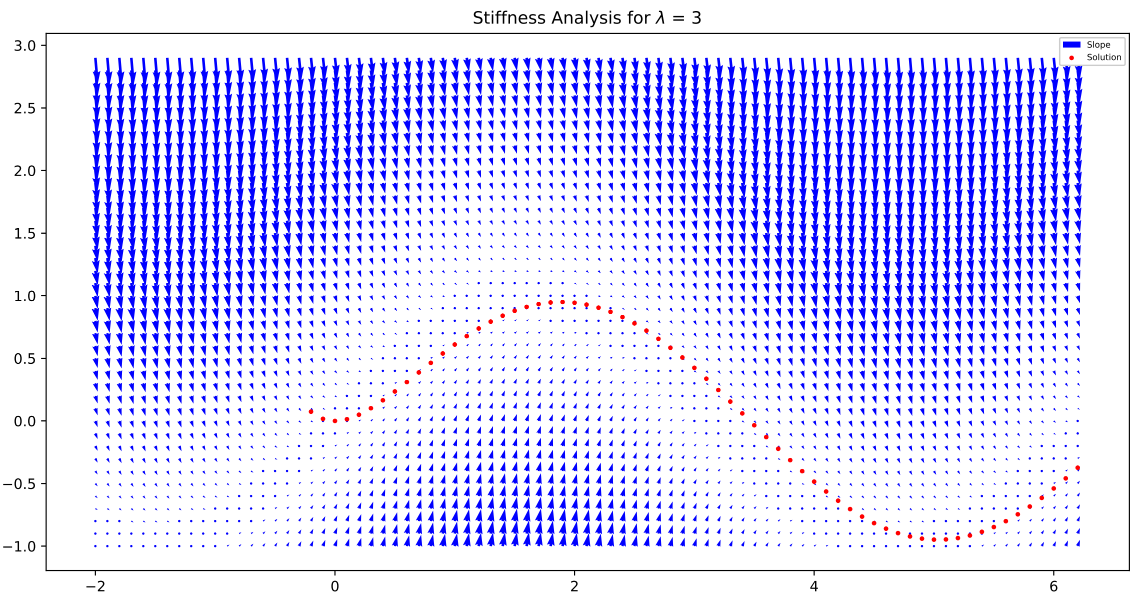

Figure 1: Variation in slope along the solution for $\lambda = 3$

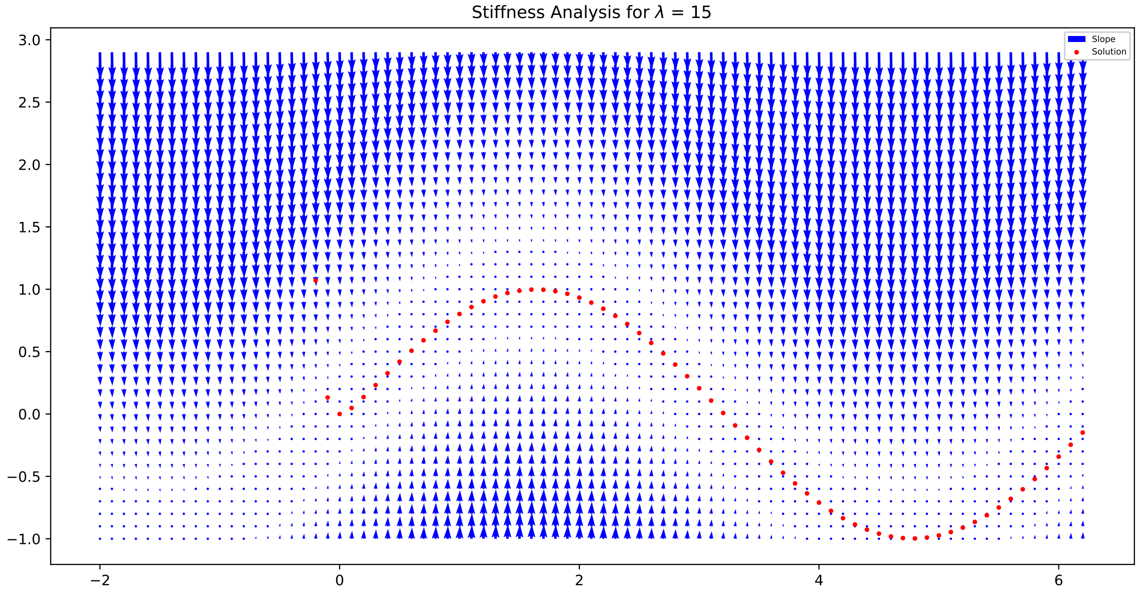

Figure 2: Variation in slope along the solution for $\lambda = 11$

The figures 1 and 2 show the dependence of slope with λ. Also, for higher values of λ, derivatives of values close to the solution of $sin(x)$ are quite small and easier to approximate, while the derivatives being large for nearby values of solution of $sin(x)$, problem in approximating appropriate solution arises. It is clear from the figure 2 that the solution of the differential equation lies in the region with wide range of the magnitude of derivatives.

2 Mathematical Modeling

Trapezoidal rule of integration is used for solving the stiff equations. This method is second order accurate. Mathematical form of the trapezoidal method is presented in equation (3). Close inspection of the equation (3) reveals that it should be solved implicitly because y_{k+1}, solution of next step, depends on itself.

$$x_{k+1} = x_k + h$$

$$y_{k+1} = y_k + \frac{h}{2}(f_{ode}(x_k, y_k) + f_{ode}(x_{k+1}, y_{k+1})) \tag{3}$$

So, we have equation of the form $F(Y_1, Y_2, ...) = 0$ which can be solved by using Newton's method.

$$F(Y_1, Y_2, ...) = F(x, y) = y - y_k - \frac{h}{2}(f_{ode}(x_k, y_k) + f_{ode}(x, y)) = 0 \tag{4}$$

Taylor series expansion, only first two terms, of the function (4) gives

$$F(x + \delta_x, y + \delta_y) = F(x, y) + \frac{\partial F}{\partial x}dx + \frac{\partial F}{\partial y}dy$$

To satisfy equation (4) we must have $F(x + \delta_x, y + \delta_y) = 0$. Thus we get an algebraic equation (5).

$$[Y_1^{n+1}, Y_2^{n+1}, ...] - [Y_1^n, Y_2^n, ...] = -(J^n)^{-1}F(Y_1^n, Y_2^n, ...) \tag{5}$$

where J^n denotes the partial derivative of F evaluated at Y^n. In the case that Y is a vector, the partial derivative must be interpeted as the Jacobian matrix,with components defined as in equation (6)

$$J_i = \frac{\partial F}{\partial Y_i} \tag{6}$$

The superscript n is used here to distinguish the iteration number, n, from the step number, k. Newton's method (usually) converges quite rapidly, so that only a few iterations are required.

When we have found a satisfactorily approximate solution Y^{n+1} to equation (5), then we take $y_{k+1} = Y^{n+1}$ and proceed with the implicit Trapezoidal method of equation (3) to get the solution y_{k+1}. Think of each of the values Y^{n+1} as successive corrections to y_{k+1}.

3 Conclusion

The method described here can be used to solve the progression of chemical reactions. Comparison of the results for reaction progression of hydrogen gas is shown in figure 3 which was solved using the same solver described here.

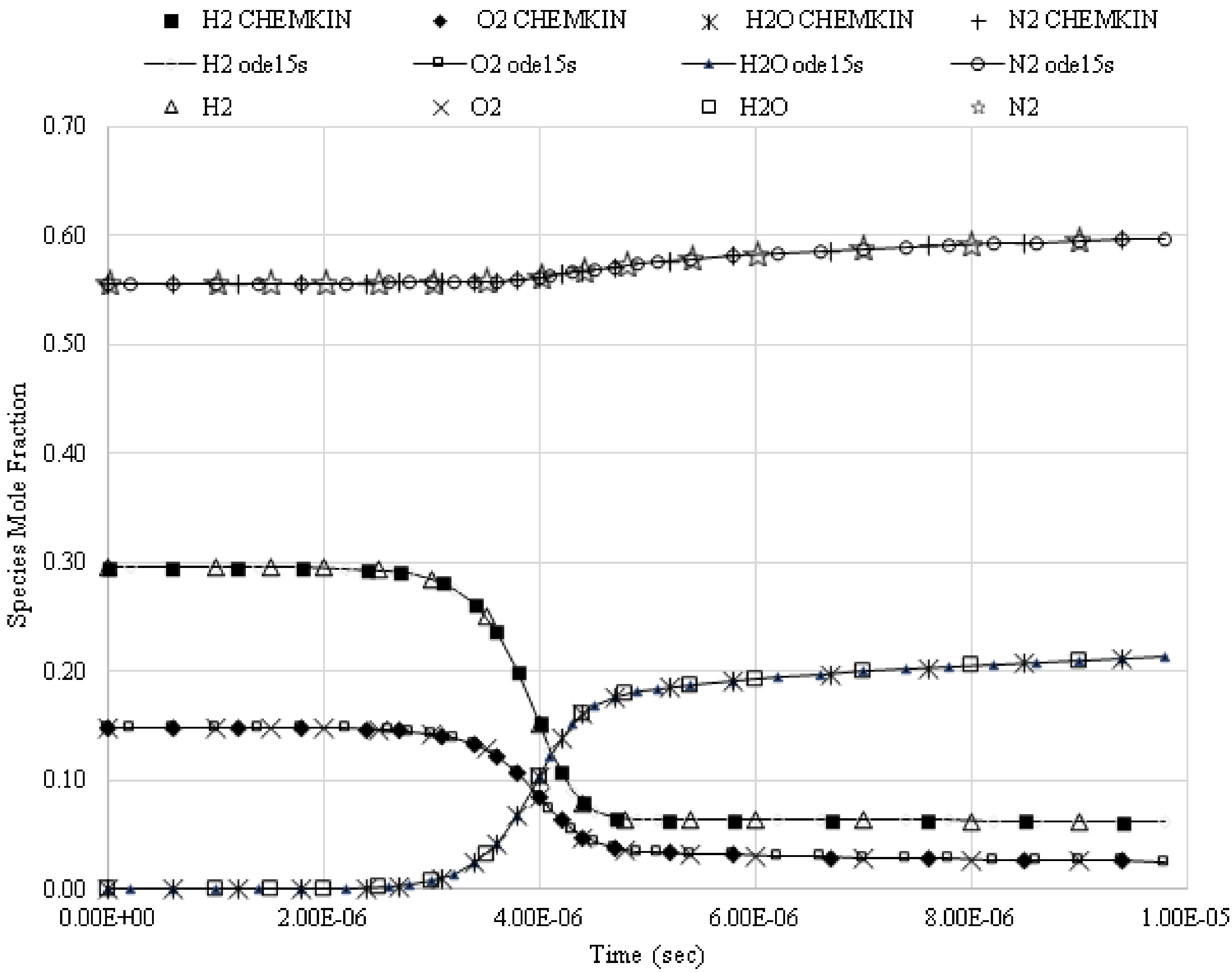

Figure 3: Variation of major species' mole fraction with time for ϕ=1, 1500 K, 2.95 atm, hydrogen-air mixture

References

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