Explicit Runge Kutta Methods

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December 16, 2016

Outline

1. Obstables
   - How to Solve ODEs, PDEs Practically/Generally
   - Accuracy and Efficiency in Numerical Schemes
2. Explicit Runge Kutta Methods
   - General Form of Explicit Runge Kutta Method
   - Practical Problems (Stiffness)
3. Adaptive Time Steps Algorithm (explicit RK)
4. Applications

Solve ODEs and PDEs analytically vs. numerically.

- "There is **no general theory known** concerning the **solvability of all partial differential equations**. Such a theory is **extremely unlikely to exist**, given the rich variety of physical, geometric, and probabilistic phenomena which can be modeled by PDE." - L. C. Evans.

- **Numerical solutions** are usually assigned to physical situations and as a result **require a lot of background information** on the type of DEs in order to solve.

Accuracy and Efficiency.

Although we can solve ODEs and PDEs numerically, many practical problems rise then.

Accuracy and Efficiency Problems

Accuracy and **efficiency** in a particular numerical scheme.

- Partial differentials and systems can be solved with **FDM, FVM** and **FEM.**
- Most equations can be solved some level of accuracy, but are **computationally expensive - lots of processing time (Efficiency Problems).**

and especially **Stiffness Problems.**

Stiffness Problems.

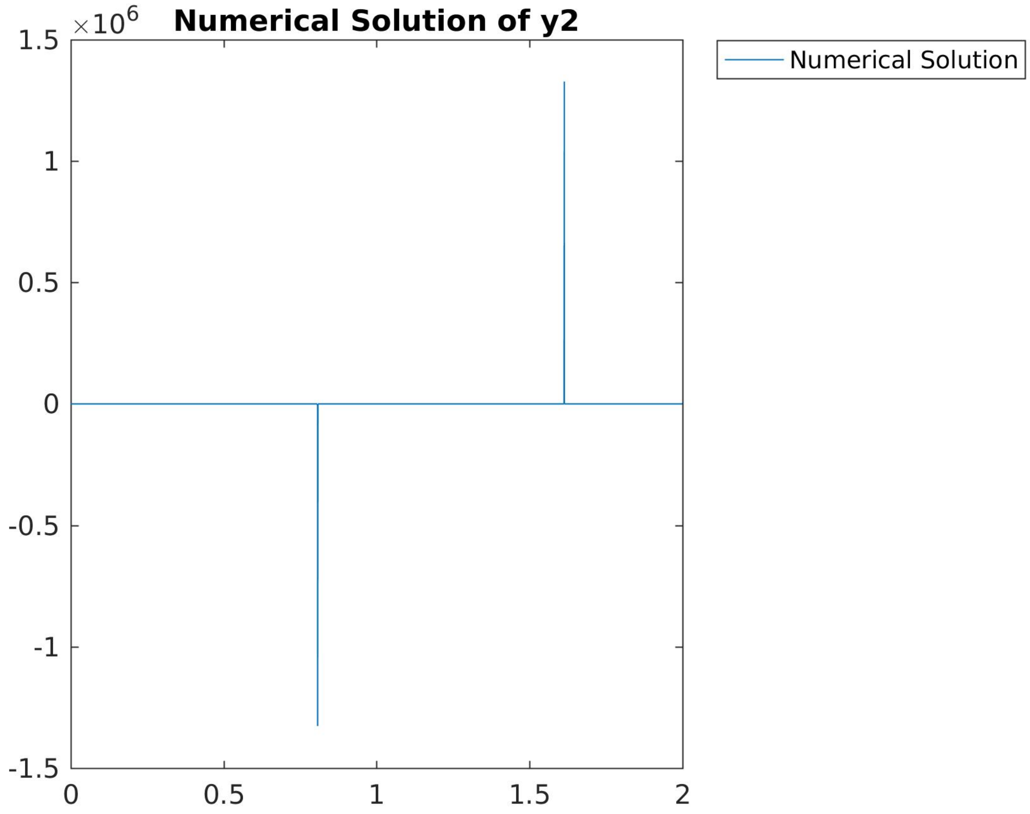

Figure 1: **Stiffness Problems.**

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- **Classic, popular, well-known** methods.
- Are a family of **explicit and implicit iterative methods** for the approximate solutions of ODEs.
- **Extremely powerful tools** for the solution of ODEs.
- One can solve a **majority of ODEs** using a Runge-Kutta scheme.

Definition of explicit Runge Kutta methods.

The family of explicit Runge Kutta methods is given by

$$y^{(n+1)} = y^{(n)} + h \sum_{i=1}^{s} b_i k_i \tag{2.1}$$

where $k_i = f(\tau_i, \eta_i), i = 1, 2, \ldots, s$ with

$$\tau_i = t_n + c_i h \tag{2.2}$$

$$\eta_i = y_n + \sum_{j=1}^{i-1} a_{ij} k_j \tag{2.3}$$

Notations. s (the number of stages), $a_{ij}, 1 \leq j < i \leq s$, b_i, $i = 1, 2, \ldots, s$ and $c_i, i = 2, 3, \ldots, s$ (the coefficients), $A = [a_{ij}]$ (the Runge Kutta matrix) and b_i (weights), c_i (nodes).

Butcher Tableau.

Consistent Runge Kutta method

The Runge Kutta method is **consistent** if

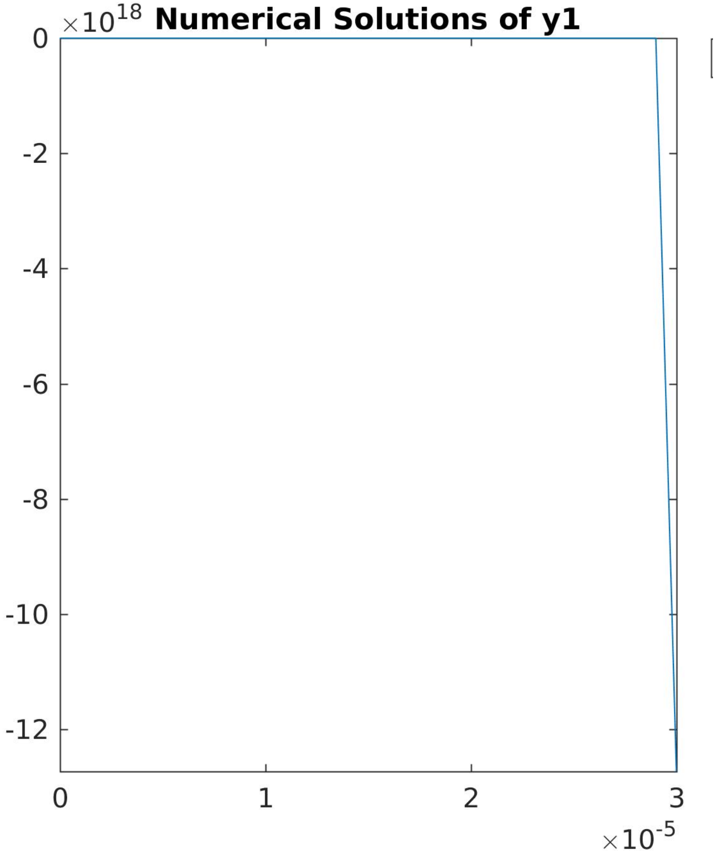
$$\sum_{j=1}^{i-1} a_{ij} = c_i, i = 2, \ldots, s \tag{2.4}$$

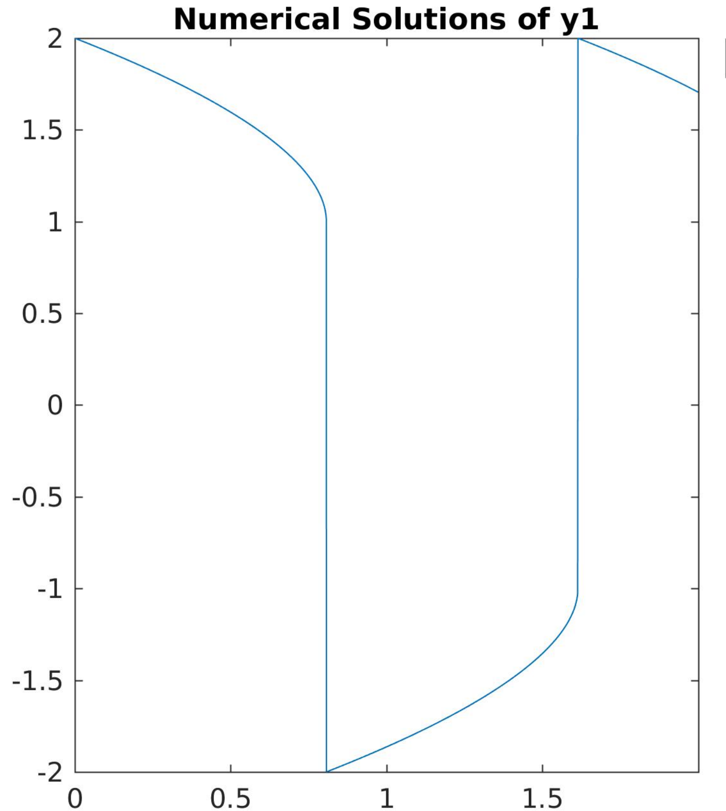
Butcher tableau.

These data are usually arranged in a **Butcher tableau.**

$$\begin{array}{c|ccccc} 0 & & & & & \\ c_2 & a_{21} & & & & \\ c_3 & a_{31} & a_{32} & & & \\ \vdots & \vdots & \vdots & \ddots & & \\ c_s & a_{s1} & a_{s2} & \cdots & a_{s,s-1} & \\ \hline & b_1 & b_2 & \cdots & b_{s-1} & b_s \end{array} \tag{2.5}$$

van der Pol Stiffness Problem.





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An Adaptive Time Step Algorithm.

- Adaptive Time Steps Scheme is **not well-known.**
- There are **lots of Adaptive Time Step Schemes.**
- An adaptive time steps algorithm for explicit Runge Kutta method can be found in the following article.

Article.

Tan Trung Nguyen, Frédérique Laurent, Rodney Fox, Marc Massot. *Solution of population balance equations in applications with fine particles: mathematical modeling and numerical schemes.* 2016. <hal-01247390v2>

Applications. Used to test numerical methods for the solution of ODEs.

Curtiss-Hirchfelder equation.

$$\frac{dy}{dt} = -50\left(y - \cos\left(t\right)\right) \tag{4.1}$$

$$y\left(0\right) = 1 \tag{4.2}$$

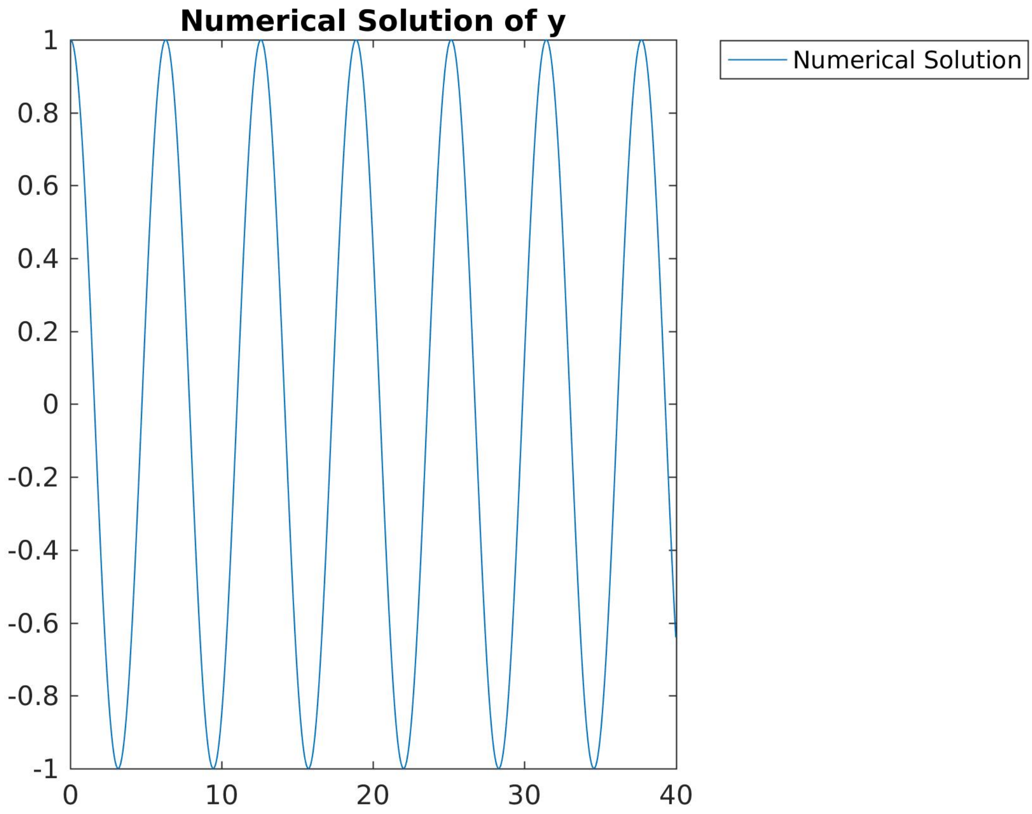

Figure 2: Using Adaptive Time Steps for Curtiss-Hirschfelder equation.

Applications.

- A theoretical model for a type of **autocatalytic reaction.**

Brusselator.

$$\frac{dy_1}{dt} = 1 - 4y_1 + y_1^2 y_2 \tag{4.3a}$$

$$\frac{dy_2}{dt} = 3y_1 - y_1^2 y_2 \tag{4.3b}$$

where $y_1(0) = 1$ and $y_2(0) = 1$.

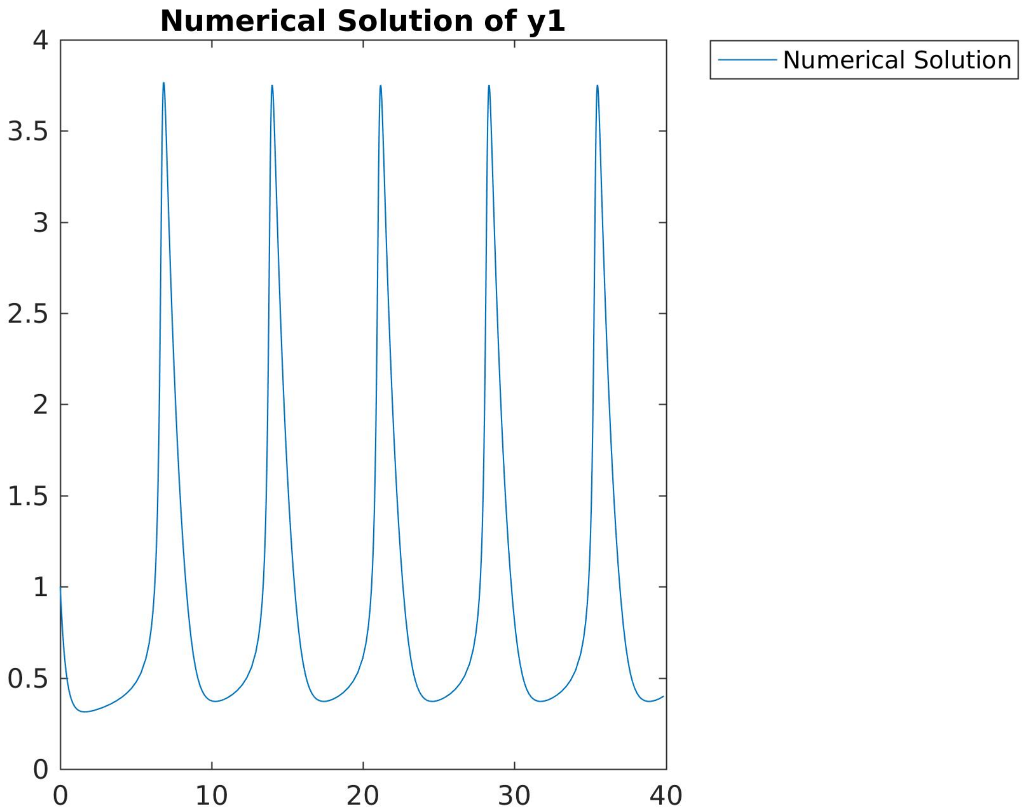

Figure 3: Using Adaptive Time Steps for Curtiss-Hirschfelder equation.

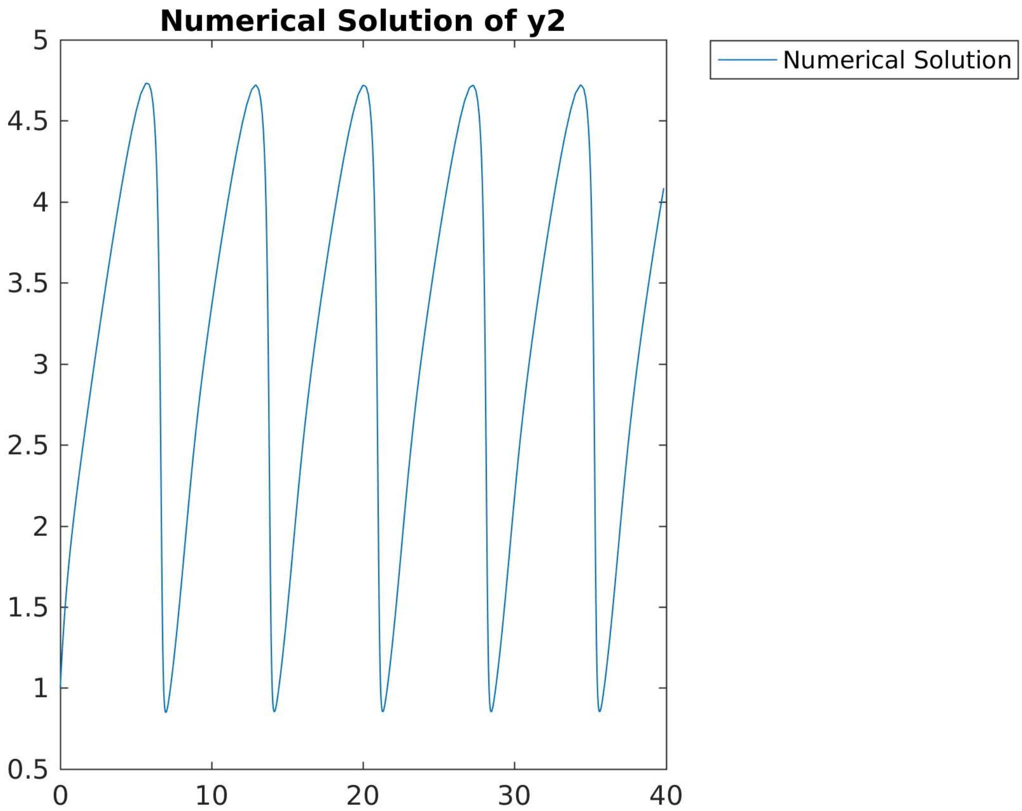

Figure 4: Using Adaptive Time Steps for Curtiss-Hirschfelder equation.

Applications.

- A classical example of **non-equilibrium thermodynamics**, resulting in the establishment of a **nonlinear chemical oscillator**.
- An interesting chemical model of **nonequilibrium biological phenomena**.
- **Mathematical models of the BZ reactions** are of theoretical interest and simulations.

Belousov-Zhabotinsky reaction (BZ) 2 ODEs

$$\frac{dy_1}{dt} = \frac{1}{\epsilon}\left(y_1(1-y_1) + f y_2 \frac{q-y_1}{q+y_1}\right) \tag{4.4a}$$

$$\frac{dy_2}{dt} = y_1 - y_2 \tag{4.4b}$$

where the coefficients are given by $f = 2/3$, $q = 8 * 10^{-4}$ and $\epsilon = 4 * 10^{-2}$.

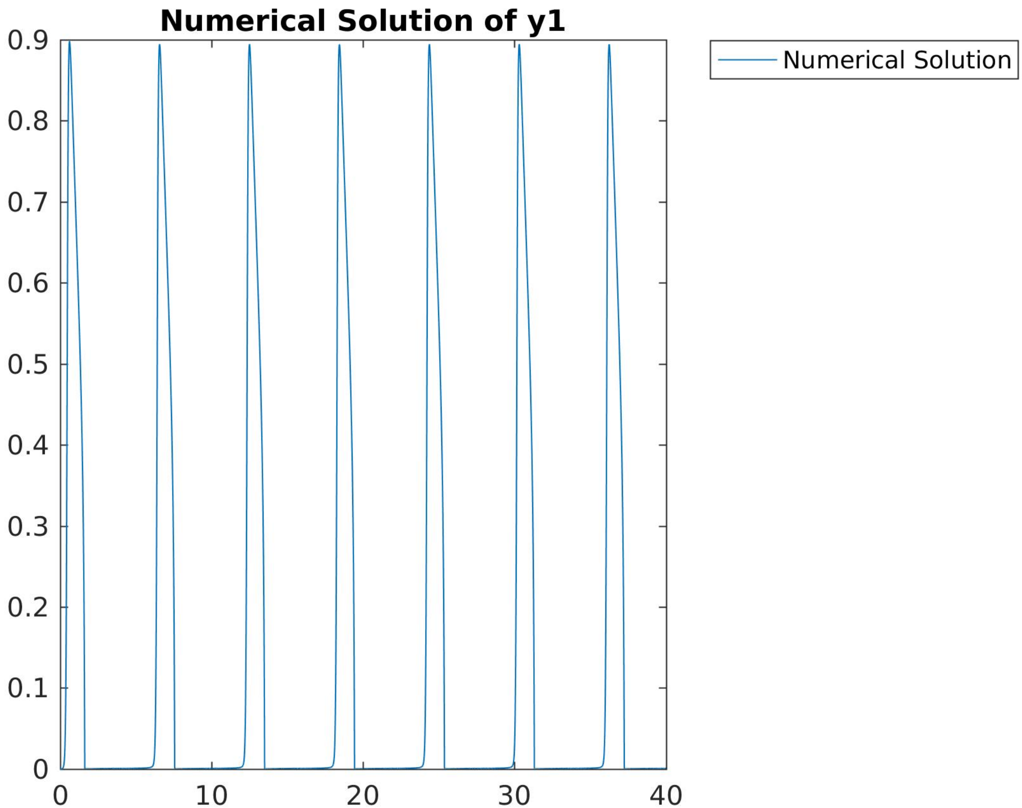

Figure 5: Using Adaptive Time Steps for Curtiss-Hirschfelder equation.

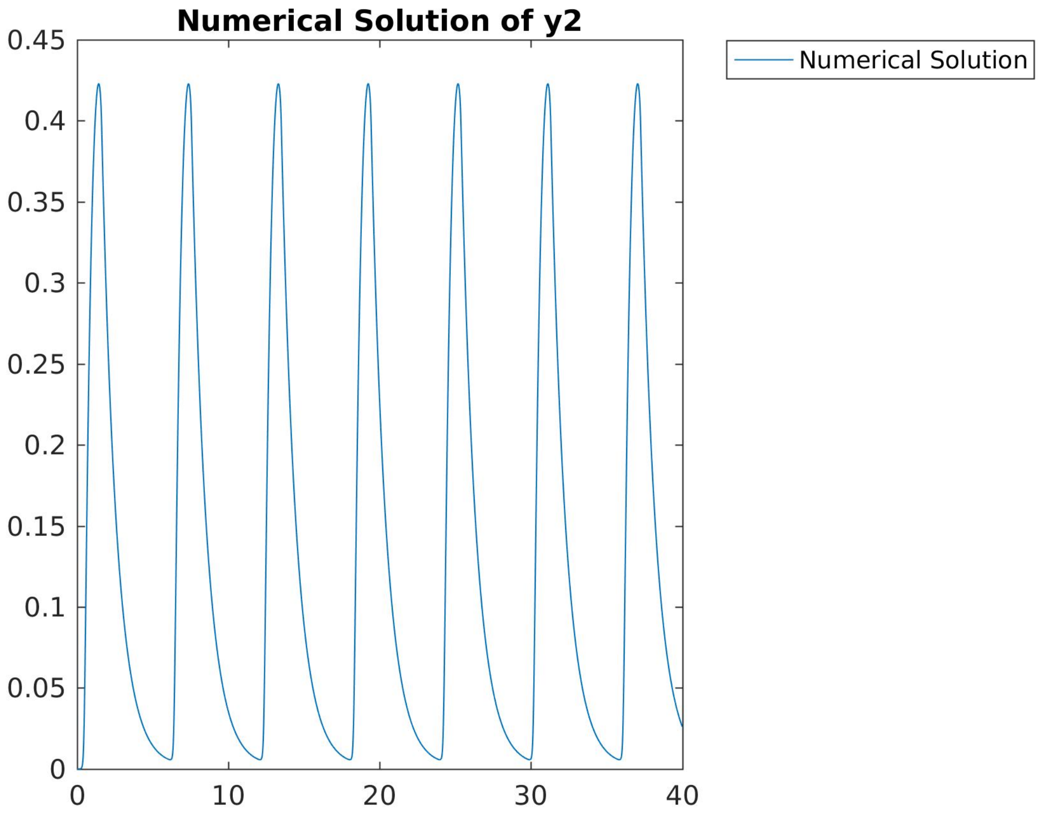

Figure 6: Using Adaptive Time Steps for Curtiss-Hirschfelder equation.

Applications.

- A theoretical model for a type of **autocatalytic reaction.**
- The simplest realistic model of the **chemical dynamics** of the **oscillatory Belousov-Zhabotinsky reaction.**
- A **reduced model of the FKN mechanism** (developed by Richard Field, Endre Körös, and Richard M. Noyes).

Oregonator.

$$\frac{dy_1}{dt} = 77.27\left[y_2 + y_1(1 - 8.375 * 10^{-6} y_1 - y_2)\right] \tag{4.5a}$$

$$\frac{dy_2}{dt} = \frac{y_3 - (1 + y_1)y_2}{77.27}, \qquad \frac{dy_3}{dt} = 0.161(y_1 - y_3) \tag{4.5b}$$

where $y_1(0) = 1$, $y_2(0) = 2$ and $y_3(0) = 3$.

Belousov-Zhabotinsky reaction (BZ) 3 ODEs

$$\frac{dy_1}{dt} = \frac{1}{\mu}(-qy_1 - y_1y_2 + fy_3) \tag{4.6a}$$

$$\frac{dy_2}{dt} = \frac{1}{\epsilon}(qy_1 - y_1y_2 + y_2 - y_2^2) \tag{4.6b}$$

$$\frac{dy_3}{dt} = y_2 - y_3 \tag{4.6c}$$

where $y_1(0) = 10$, $y_2(0) = 0.04$, $y_3(0) = 0.1$, where the coefficients are given by $f = 2/3$, $q = 8 * 10^{-4}$, $\mu = 10^{-6}$ and $\epsilon = 4 * 10^{-2}$.

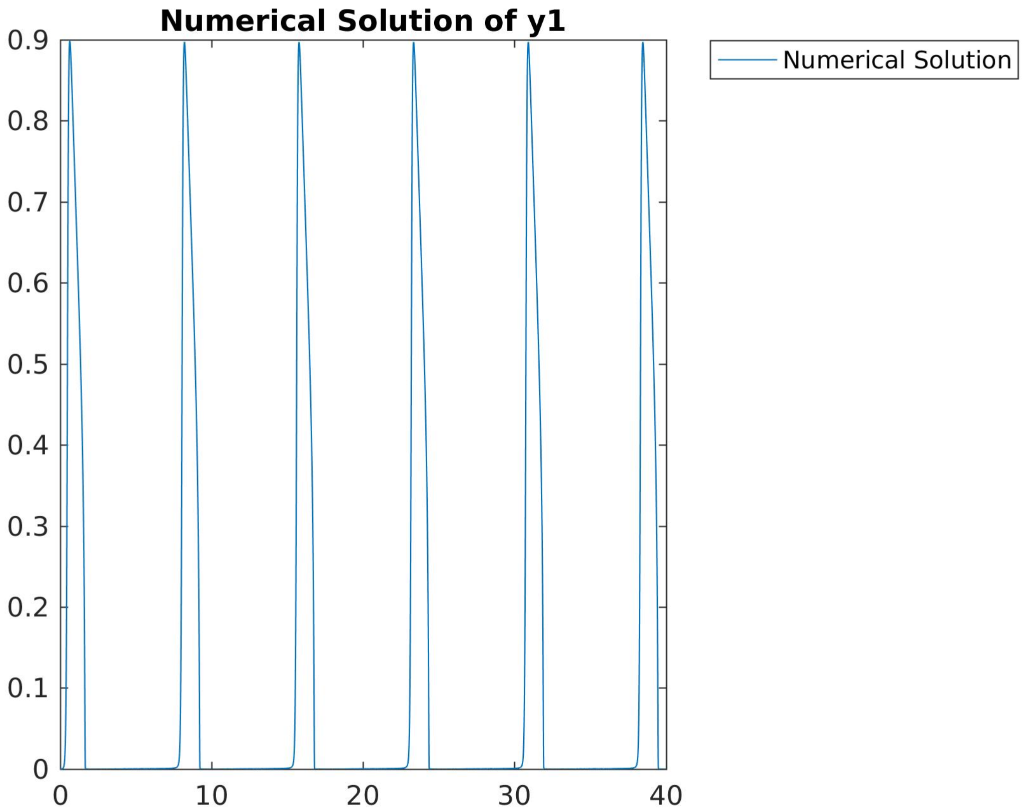

Figure 7: Using Adaptive Time Steps for Curtiss-Hirschfelder equation.

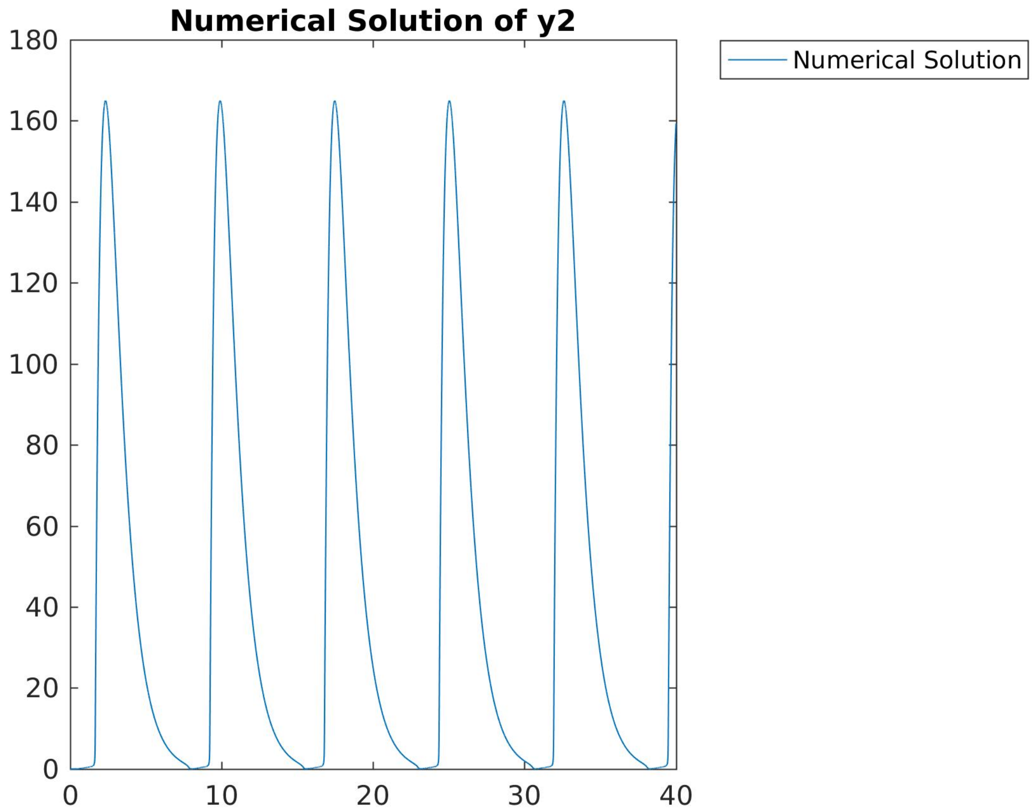

Figure 8: Using Adaptive Time Steps for Curtiss-Hirschfelder equation.

Applications. A basic model for **oscillatory processes** in physics, electronics, biology, neurology, sociology and economics

- **Physics.** Models **electrical circuits connected with triod oscillators**. A prototype for systems with **self-excited limit cycle oscillations.**
- **Medicine.** Study the range of **stability of heart dynamics.** Situation in which a real heart is driven by a pacemaker. Stabilize a **heart's irregular beating.**
- **Biology.** The basis of a model of **coupled neurons in the gastric mill circuit** of the **stomatogastric ganglion**
- **Seismology.** Used in the development a model of the **interaction of two plates** in a **geological fault.**

van der Pol equations

$$\frac{dy_1}{dt} = y_2 \tag{4.7a}$$

$$\frac{dy_2}{dt} = [(1 - y_1^2)y_2 - y_1]/\epsilon \tag{4.7b}$$

where $\epsilon = 10^{-6}$.

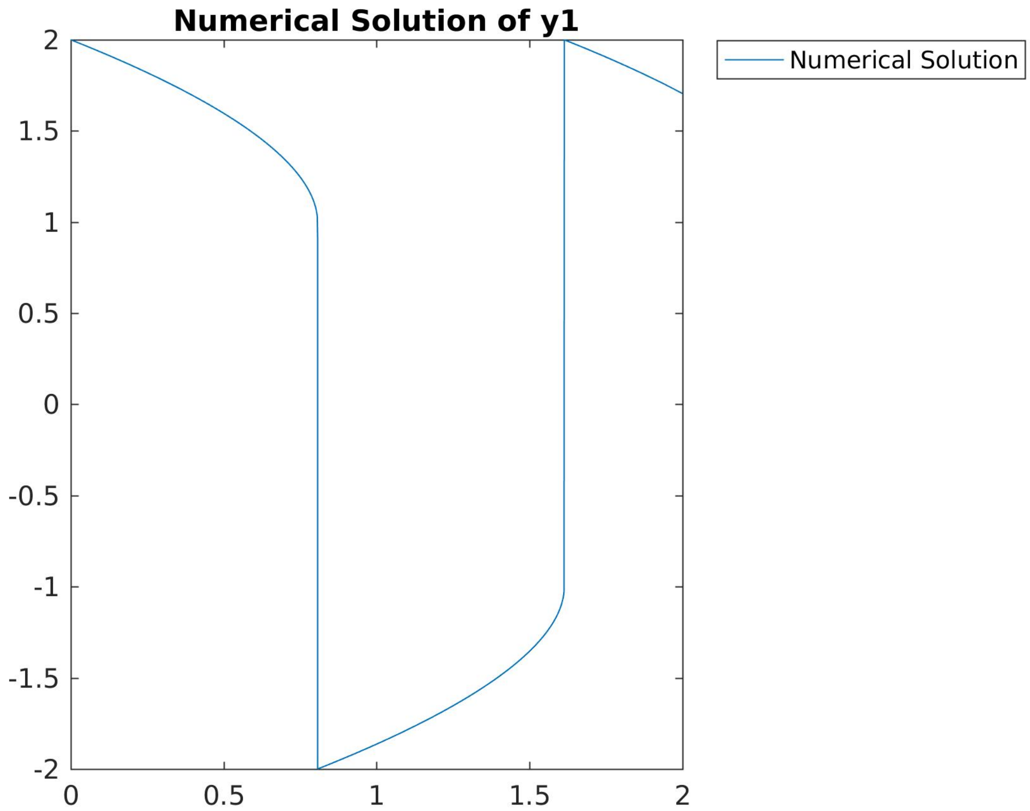

Figure 9: Using Adaptive Time Steps for Curtiss-Hirschfelder equation.

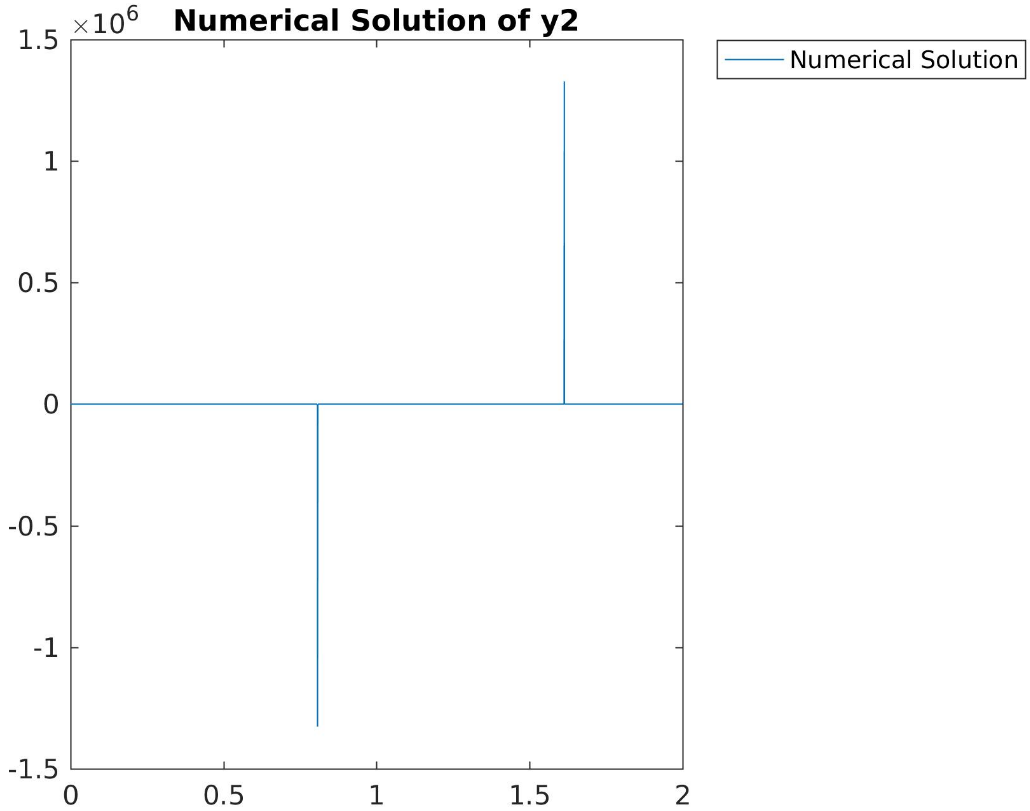

Figure 10: Using Adaptive Time Steps for Curtiss-Hirschfelder equation.

References

Tan Trung Nguyen, Frédérique Laurent, Rodney Fox, Marc Massot. *Solution of population balance equations in applications with fine particles: mathematical modeling and numerical schemes*. 2016. <hal-01247390v2>