0.1 Introduction

0.2 Stability diagrams: graphical representations and their use

0.2.1

Figure 1 shows the stability diagram of Runge Kutta schemes of order 1, 2, 3 and 4. Generally speaking, the stability domain size increases with the order of the scheme. For the higher-order scheme, the real part of z being positive means that the numerical scheme may converge whereas the system will diverge for such z (for example for a solution which form is : $e^{\lambda t}$).

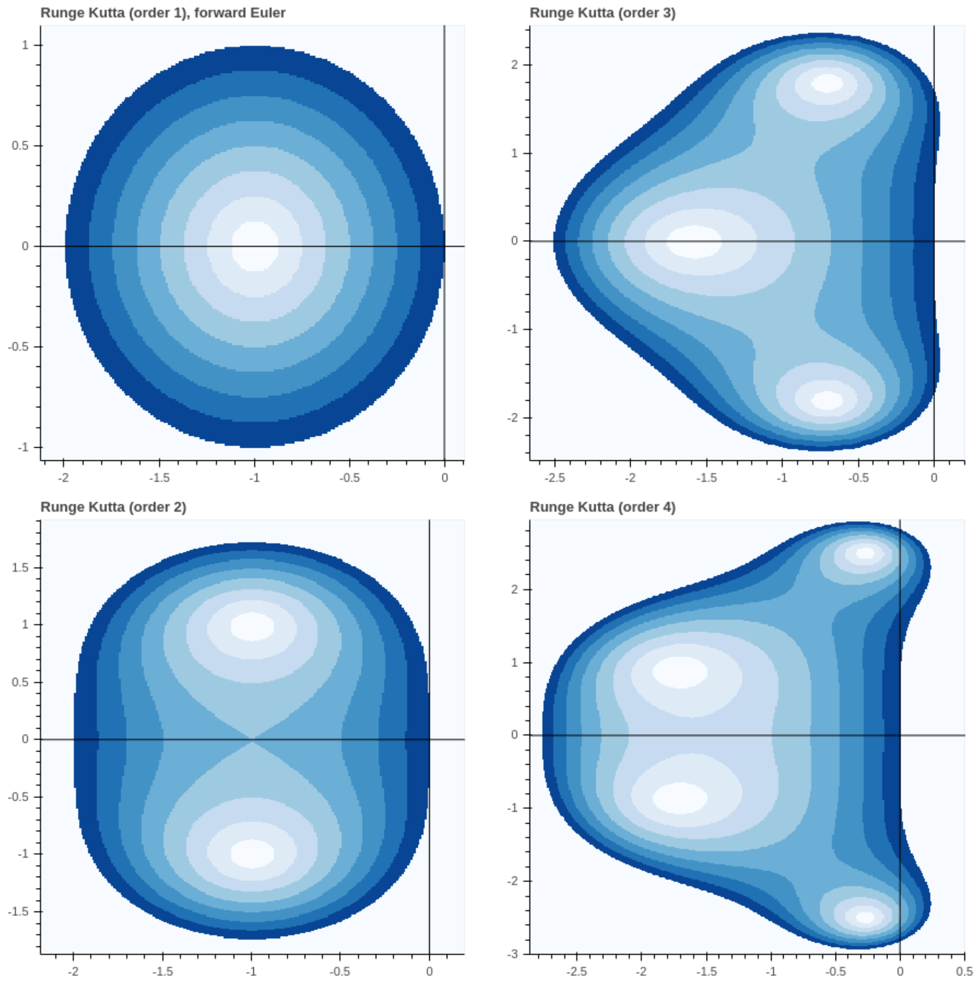

Figure 1: Stability diagrams for Runge Kutta schemes of order : 1, 2, 3 and 4 (left to right, top to bottom). The stability domain increases with the order. However, stability to some eigen values with positive real part occurs for order 3 and 4 schemes. This means that while the system diverges for such eigen values, the scheme will remain stable and converge.

0.2.2

Choosing a time step close to the boundary but still in the stability domain of the scheme meant having oscillations for the Curtiss and Hirschfelder model. An example is given in figure 2.

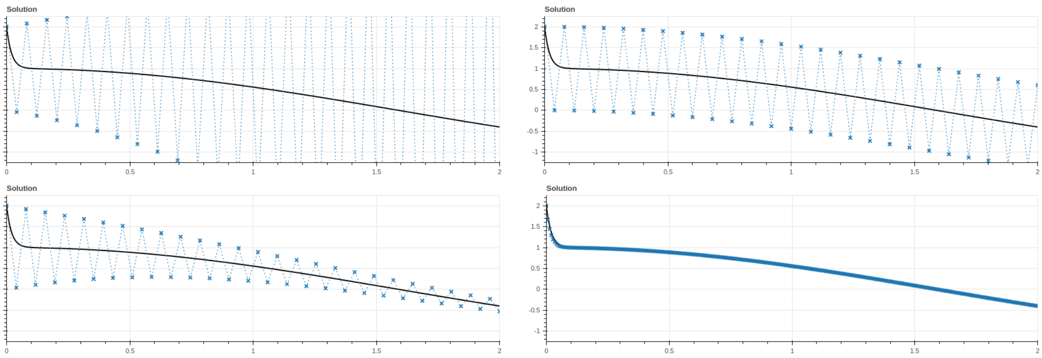

Figure 2: Examples of the Curtiss and Hirschfelder model for $k = 50$, $T = 2$ sec and $n_t = 50, 51, 52, 300$ (left to right, top to bottom). The first example shows a diverging scheme, n_t was choosen too little. The second example, with $n_t = 51$, seems like the scheme is right on its stability boundary, as oscillations are neither decayed nor amplified. The two following ones show the scheme bahavior close to the boundary ($n_t = 52$, lots of oscillations) and far from it ($n_t = 300$, no oscillations).

Stablity and accuracy are two distincts notions (as figure 2 shows). One stable scheme may be far from the solution even if it should converge for $t >> 1$. A unstable scheme will never be accurate however.

0.3

The figure 3 shows the stability domain of the DOPRI methods.

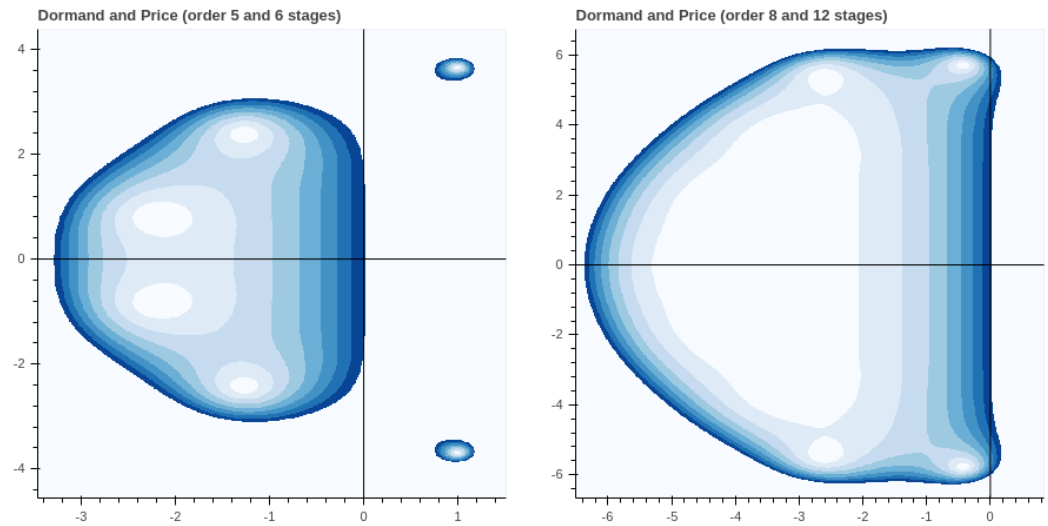

Figure 3: In comparison with the RK schemes, these schemes allow for bigger negative eigen values real part (-3.2 and -6.2 *vs* -2.8 at best previously. DOPRI schemes also cover a bigger imaginary axis that the RK schemes. One should be careful not to have system eigen values z with $\Re(z) > 0$ that falls in the stability domain.