# Fundamentals of Simulation Methods

University of Heidelberg, WiSe 2021/2022

Mandatory assignements - Set 2

**Authors:** Matteo Zortea, Anja Heim

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## Exercise 1

We consider a simple differential equation of the form

$$\frac{dy}{dt} = f(y) \tag{1}$$

which is to be integrated with an explicit midpoint method as follows:

$$y^{n+1} = y^n + \Delta t f\left(y^n + \frac{\Delta t}{2} f(y^n, t_n), t_n + \frac{\Delta t}{2}\right). \tag{2}$$

To determine its accuracy order, we look at the difference $y^{n+1} - y(t_n + \Delta t)$, i.e. between the approximate and the exact function value after one step. By using Taylor expansion, we get

$$\begin{aligned} y^{n+1} - y(t_n + \Delta t) = \\ &= y^n + \Delta t f\left(y^n + \frac{\Delta t}{2} f(y^n, t_n), t_n + \frac{\Delta t}{2}\right) - \left[y^n + \frac{dy}{dt}|_n \Delta t + \frac{1}{2}\frac{d^2y}{dt^2}|_n \Delta t^2 + O(\Delta t^3)\right] = \\ &= \Delta t f(y^n, t_n) + \frac{\Delta t^2}{2}\frac{\partial f}{\partial t}|_n + \frac{\Delta t^2}{2}\frac{\partial f}{\partial y}\frac{\partial y}{\partial t}|_n + O(\Delta t^3) - \Delta t f(y^n, t_n) - \frac{\Delta t^2}{2}\frac{d^2y}{dt^2}|_n + O(\Delta t^3) = \\ &= O(\Delta t^3). \end{aligned} \tag{3}$$

We used that $\frac{\Delta t^2}{2}\frac{\partial f}{\partial t}|_n + \frac{\Delta t^2}{2}\frac{\partial f}{\partial y}\frac{\partial y}{\partial t}|_n = \frac{\Delta t^2}{2}\frac{df}{dt}|_n$ and $\frac{d^2y}{dt^2}|_n = \frac{df}{dt}|_n$.

This means the local truncation error is of the order

$$\epsilon_{loc} = O(\Delta t^3). \tag{4}$$

The global truncation error averaged over all timesteps is thus

$$\epsilon_{glob} = \frac{\epsilon_{loc}}{\Delta t} = O(\Delta t^2). \tag{5}$$

This explicit midpoint method is as we see of second-order accuracy in the time step $\Delta t$.

## Exercise 2

The temperature evolution of an ionized plasma of hydrogen gas is given as

$$\frac{dT}{dt} = -\frac{2}{3k_B} n_H \Lambda(T), \tag{6}$$

where $k_B = 1.38 \times 10^{-23} JK^{-1}$ is the Boltzmann constant, $n_H = 10^6 m^{-3}$ is the (here fixed) density of hydrogen atoms, and the cooling rate $\Lambda(T)$ is given as

$$\Lambda(T) = \begin{cases} \Lambda_0 \left(\frac{T}{T_0}\right)^{\alpha} & for \;\; T \leq T_0 \\ \Lambda_0 \left(\frac{T}{T_0}\right)^{\beta} & for \;\; T > T_0 \end{cases} \tag{7}$$

with $\Lambda_0 = 10^{-35} J m^3 s^{-1}$, $\alpha = 10.0$, $\beta = -0.5$ and $T_0 = 2 \times 10^4 K$.

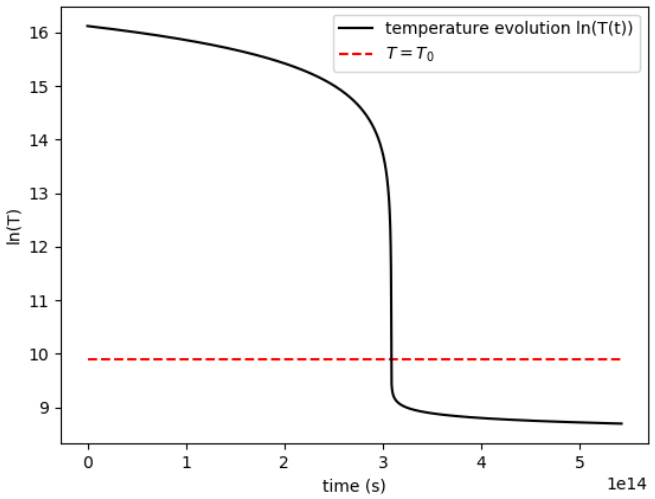


Figure 1: Time evolution in logarithmic scale $ln(T(t))$ for a step size $\Delta t = 10^{10} s$.

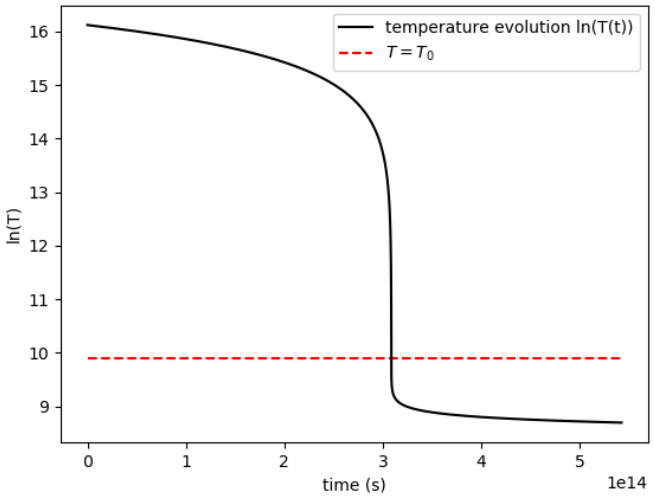


Figure 2: Time evolution in logarithmic scale $ln(T(t))$ for a step size $\Delta t = 8.8 \times 10^{10} s$.

## a)

Using a second-order explicit Runge-Kutta predictor-corrector method with a time step of $\Delta t = 10^{10} s$ and starting at an temperature $T_{init} = T(t = 0) = 10^7 K$, the temperature evolution until $T < 6 \times 10^3 K$ is plotted in fig. 1 with the temperature in logarithmic scale. Using this time step size, the chosen integration scheme takes 54237 steps until it reaches the desired temperature. The dashed red horizontal line marks the point when the temperature drops below the threshold $T_0 = 2 \times 10^4 K$ and one clearly sees the change in the curvature in this point related to the switch in the exponent of the cooling rate (7).

## b)

As said, it takes 54237 steps at a time step size of $\Delta t = 10^{10} s$ for the temperature to drop from $T_{init} = 10^7 K$ to $T = 6000 K$.

The number of steps can be decreased by enlarging $\Delta t$, for a time step size of $\Delta t = 8.8 \times 10^{10} s$ for example, the output plot still looks the same, see fig. 2, only needing 6164 steps. But at $\Delta t = 9 \times 10^{10} s$ (3431 steps), the method somehow fails, resulting in an image as can be seen in fig. 3, where the time step size is too big to represent the curvature switch at $T = T_0$ and simply drops below $T = 6000 K$.

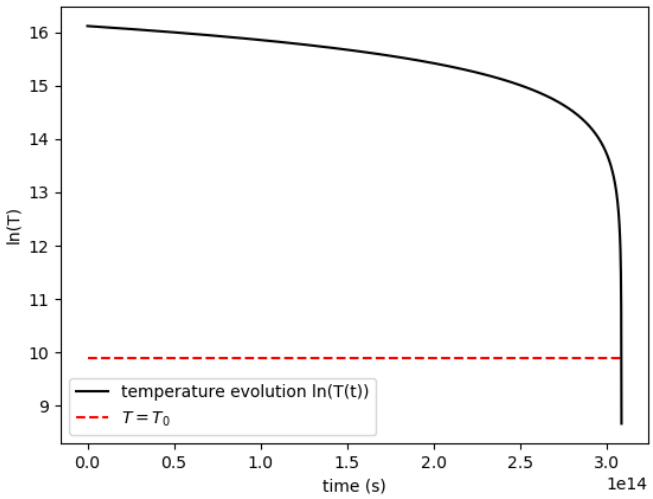


Figure 3: Time evolution in logarithmic scale $ln(T(t))$ for a step size $\Delta t = 9 \times 10^{10} s$.

## c)

We have then improved the algorithm using an adaptive stepsize. The results are reported in the following 3 plots, and compared to one obtained for the fixed stepsize. The adaptive stepsize improves a lot the

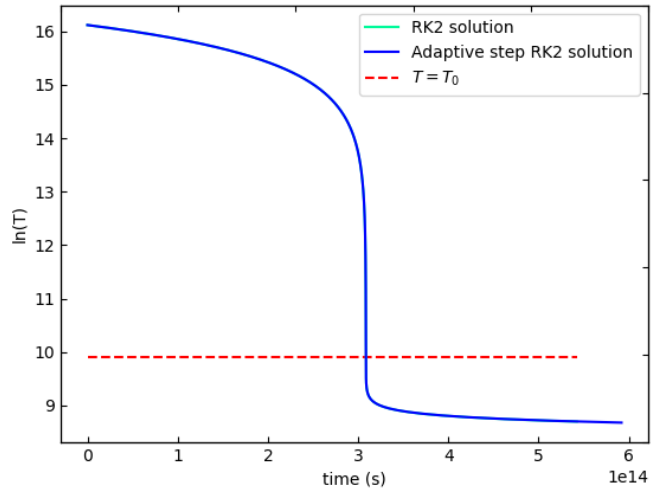


Figure 4: Comparison between adaptive stepsize integration (blue) and fixed stepsize (green) Both methods were started with a stepsize of value $\Delta t = 10^{10}$ s

speed of the algorithm. Indeed only $337 \pm 1$ steps are needed for the adaptive stepsize algorithm, quite independently of the starting stepsize. On the other side the fixed stepsize method requires at least $\sim 6000$ steps

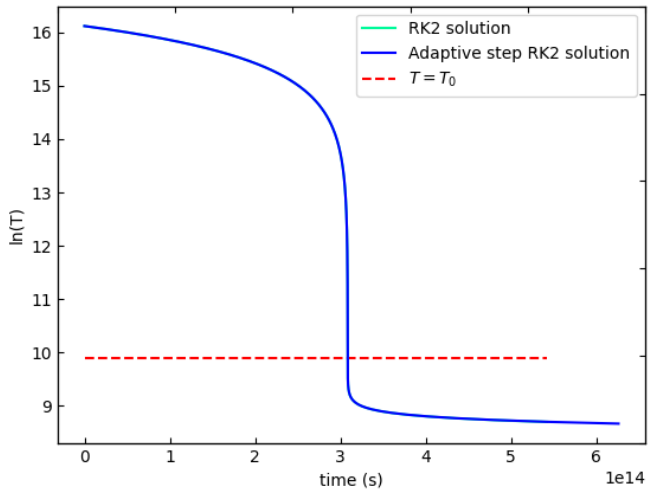


Figure 5: Comparison between adaptive stepsize integration (blue) and fixed stepsize (green) Both methods were started with a stepsize of value $\Delta t = 8.8 \times 10^{10}$ s

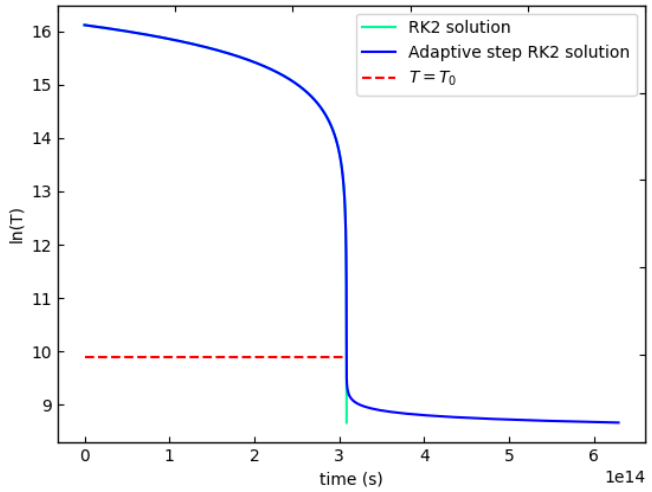


Figure 6: Comparison between adaptive stepsize integration (blue) and fixed stepsize (green) Both methods were started with a stepsize of value $\Delta t = 9 \times 10^{10}$ s

# Exercise 3

### a)

By defining

$$q_i \equiv \frac{\partial \mathcal{L}}{\dot{q}_i} \qquad i = 1, 2 \tag{8}$$

one can rewrite the Lagrangian equations of motion as

$$\frac{dq_1}{dt} = \frac{\partial \mathcal{L}}{\partial q_1} = -m_2 l_1 l_2 \dot{\phi}_1 \dot{\phi}_2 \sin(\phi_1 - \phi_2) - (m_1 + m_2) g l_1 \sin \phi_1$$
$$\frac{dq_2}{dt} = \frac{\partial \mathcal{L}}{\partial q_2} = m_2 l_1 l_2 \dot{\phi}_1 \dot{\phi}_2 \sin(\phi_1 - \phi_2) - m_2 g l_2 \sin \phi_2$$

These equations determine the evolution of the momenta $q_1, q_2$.

**b)**

If we define a state vector as $y = (\phi_1, \phi_2, q_1, q_2)T$, the evolution of our system is completely determined by the set of equations

$$\frac{dy}{dt} = f(y)$$

which, in matrix form, read

$$\begin{pmatrix} \frac{d\phi_1}{dt} \\ \frac{d\phi_2}{dt} \\ \frac{dq_1}{dt} \\ \frac{dq_2}{dt} \end{pmatrix} = \begin{pmatrix} \dot{\phi}_1 \\ \dot{\phi}_2 \\ -m_2 l_1 l_2 \dot{\phi}_1 \dot{\phi}_2 \sin(\phi_1 - \phi_2) - (m_1 + m_2) g l_1 \sin\phi_1 \\ m_2 l_1 l_2 \dot{\phi}_1 \dot{\phi}_2 \sin(\phi_1 - \phi_2) - m_2 g l_2 \sin\phi_2 \end{pmatrix} \tag{9}$$

We now need to obtain the expression for $\dot{\phi}_i \quad i = 1, 2$. In order to do this, let us explicitly write the expression for $q_1, q_2$ using their definition 8.

$$q_1 = \frac{\partial \mathcal{L}}{\partial \dot{q}_1} = (m_1 + m_2) l_1^2 \dot{\phi}_1 + m_2 l_1 l_2 \dot{\phi}_2 cos(\phi_1 - \phi_2) \equiv \alpha \dot{\phi}_1 + \beta \dot{\phi}_2$$
$$q_2 = \frac{\partial \mathcal{L}}{\partial \dot{q}_2} = m_2 l_1 l_2 \dot{\phi}_1 \cos(\phi_1 - \phi_2) + m_2 l_2^2 \dot{\phi}_2 \equiv \beta \dot{\phi}_1 + \gamma \dot{\phi}_2$$

which can be written in matrix form as

$$\begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = \begin{pmatrix} \alpha & \beta \\ \beta & \gamma \end{pmatrix} \begin{pmatrix} \dot{\phi}_1 \\ \dot{\phi}_2 \end{pmatrix}$$

We can invert these expressions using Kramer's rule

$$\dot{\phi}_1 = \frac{\begin{vmatrix} q_1 & \beta \\ q_2 & \gamma \end{vmatrix}}{\begin{vmatrix} \alpha & \beta \\ \beta & \gamma \end{vmatrix}} = \frac{\gamma}{\alpha\gamma - \beta^2} q_1 - \frac{\beta}{\alpha\gamma - \beta^2} q_2 \qquad \dot{\phi}_2 = \frac{\begin{vmatrix} \alpha & q_1 \\ \beta & q_2 \end{vmatrix}}{\begin{vmatrix} \alpha & \beta \\ \beta & \gamma \end{vmatrix}} = \frac{\alpha}{\alpha\gamma - \beta^2} q_2 - \frac{\beta}{\alpha\gamma - \beta^2} q_2$$

and by popping in the expressions for $\alpha, \beta, \gamma$

$$\dot{\phi}_1 = \frac{1}{m_1 l_1^2 (1 + m_2/m_1 \sin^2(\phi_1 - \phi_2))} q_1 - \frac{cos(\phi_1 - \phi_2)}{m_1 l_1 l_2 (1 + m_2/m_1 \sin^2(\phi_1 - \phi_2))} q_2$$
$$\dot{\phi}_2 = -\frac{1}{\mu l_2^2 (1 + m_2/m_1 \sin^2(\phi_1 - \phi_2))} q_2 - \frac{\cos(\phi_1 - \phi_2)}{m_1 l_1 l_2 (1 + m_2/m_1 \sin^2(\phi_1 - \phi_2))} q_1$$

where $\mu = \frac{m_1 m_2}{m_1 + m_2}$ is the reduced mass.
We have now obtained all the expressions needed to solve equation 9 which now explicitly reads

$$\begin{pmatrix} \frac{d\phi_1}{dt} \\ \frac{d\phi_2}{dt} \\ \frac{dq_1}{dt} \\ \frac{dq_2}{dt} \end{pmatrix} = \begin{pmatrix} \frac{1}{m_1 l_1^2 (1 + m_2/m_1 \sin^2(\phi_1 - \phi_2))} q_1 - \frac{cos(\phi_1 - \phi_2)}{m_1 l_1 l_2 (1 + m_2/m_1 \sin^2(\phi_1 - \phi_2))} q_2 \\ -\frac{1}{\mu l_2^2 (1 + m_2/m_1 \sin^2(\phi_1 - \phi_2))} q_2 - \frac{\cos(\phi_1 - \phi_2)}{m_1 l_1 l_2 (1 + m_2/m_1 \sin^2(\phi_1 - \phi_2))} q_1 \\ -m_2 l_1 l_2 \dot{\phi}_1 \dot{\phi}_2 \sin(\phi_1 - \phi_2) - (m_1 + m_2) g l_1 \sin\phi_1 \\ m_2 l_1 l_2 \dot{\phi}_1 \dot{\phi}_2 \sin(\phi_1 - \phi_2) - m_2 g l_2 \sin\phi_2 \end{pmatrix}$$

**c)**

We need an expression for the energy. There are two alternatives to do this. One is to perform the Legendre transform on $\mathcal{L}$, thus obtaining the hamiltonian of the system $\mathcal{H} = \mathcal{H}(t, \phi, q)$. The second way consists in remembering that $\mathcal{L} = T - V$ so that the energy of the system $E = E(t, \phi, \dot{\phi})$ can be obtained by flipping the sign of the potential energy in the given lagrangian. In our simulation we adopted the latter procedure.

$$E = T + V = \frac{m_1}{2} \left(l_1 \dot{\phi}_1\right)^2 + \frac{m_2}{2} \left[\left(l_1 \dot{\phi}_1\right)^2 + \left(l_2 \dot{\phi}_2\right)^2 + 2 l_1 l_2 \dot{\phi}_1 \dot{\phi}_2 \cos(\phi_1 - \phi_2)\right] +$$
$$+ m_1 g l_1 (1 - \cos\phi_1) + m_2 g \left[l_1 (1 - \cos\phi_1) + l_2 (1 - \cos\phi_2)\right]$$

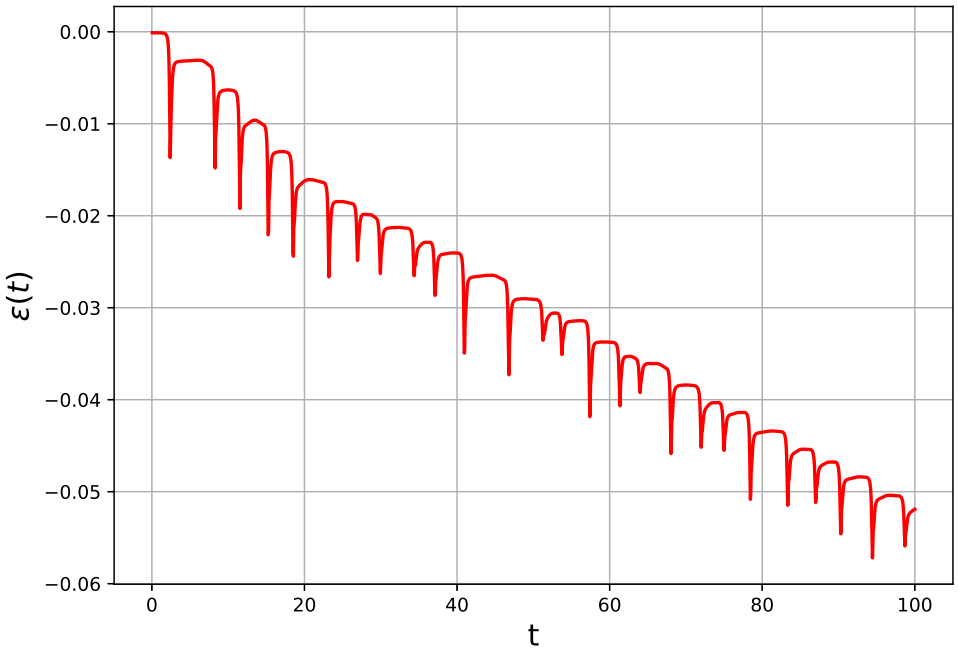


Figure 7: Energy relative error $\epsilon(t) = \frac{E(t)-E(0)}{E(0)}$ with the RK2 integrator

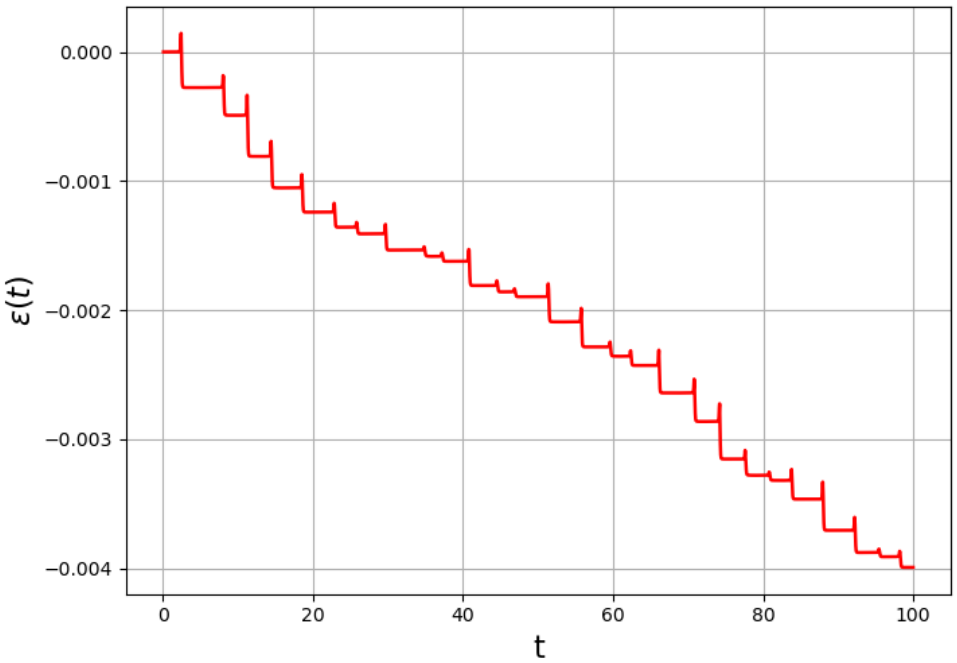


Figure 8: Relative energy error $\epsilon(t) = \frac{E(t)-E(0)}{E(0)}$ with the RK4 integrator scheme

**d)**

As can be seen in fig. 8, the relative error in the energy drops much more quickly for the RK2 scheme than for the RK4 one, which matches our expectations.

**e)**

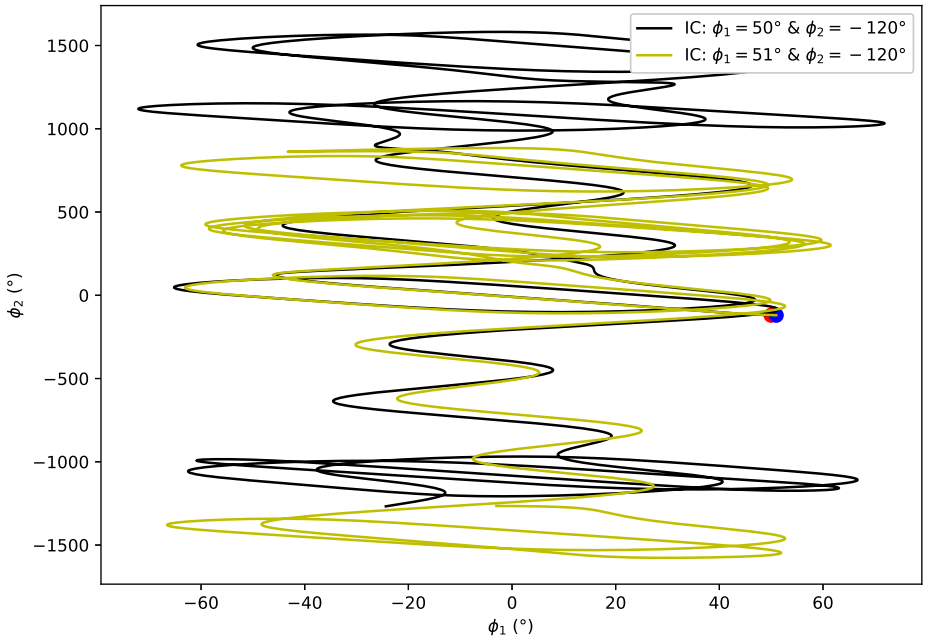


Figure 9: Plot of $\phi_2$ vs $\phi_1$. The two pendulums are started respectively with $\phi_1^{(1)} = 50°\phi_1^{(2)} = 51°$ and $\phi_2^{(1)} = \phi_2^{(2)} = -120°$

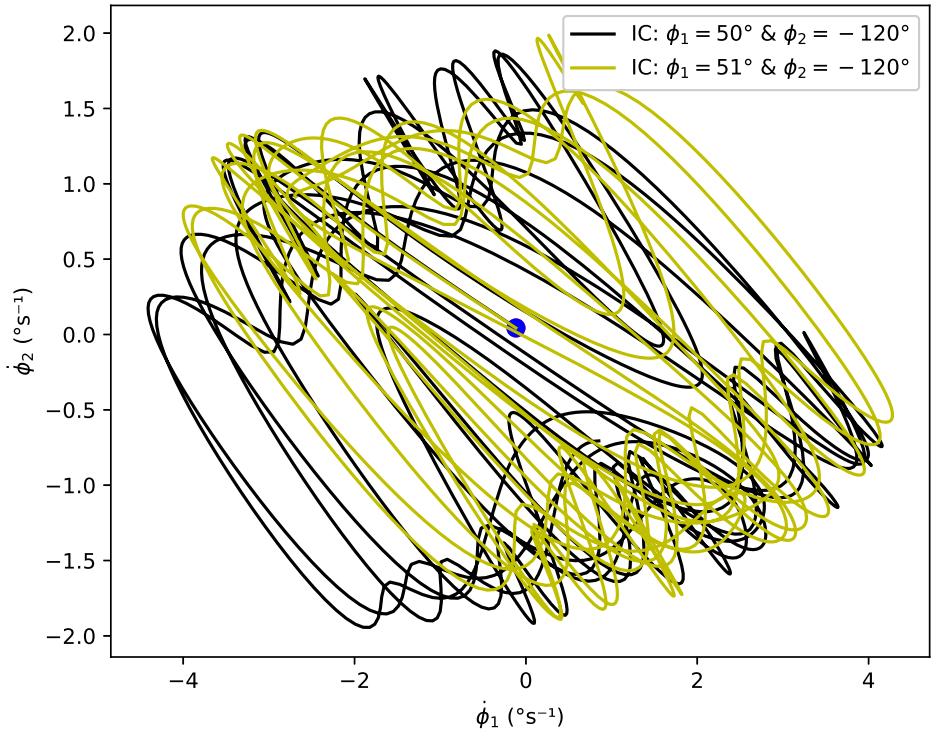


Figure 10: Plot of $\dot{\phi}_2$ vs $\dot{\phi}_1$. The two pendulums are started respectively with $\phi_1^{(1)} = 50°\phi_1^{(2)} = 51°$ and $\phi_2^{(1)} = \phi_2^{(2)} = -120°$