Project 4, Part 1 Scientific Computing 2021

Kimi Cardoso Kreilgaard (twn176)

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The HIV virus that eventually leads to AIDS is spread mainly through (i) sexual contact, (ii) transfer of blood through transfusions or (iii) the sharing of needles by drug users. In this project we will model the spread of the virus with a forward Euler method and a fourth order Runge Kutta method.

1 Considering Only Infection Through Sexual Contact

1.1 Description and Assumptions

We start out by considering the spread of the HIV virus through sexual contact where the initial group is homosexual. For simplicity (I hope), the assignment does not include bisexual or homosexual women, who could otherwise also be infected. We suppose that at time t there are in a group of individuals:

(i) p_1 homosexual males of which $x_1(t)$ are infected

(ii) p_2 bisexual males of which $x_2(t)$ are infected

(iii) q heterosexual females of which $y(t)$ are infected

(iv) r heterosexual males of which $z(t)$ are infected

We assume that the rate of infection is proportional to the number of sexual contacts and therefore we have the following set of equations:

$$\frac{dx_1}{dt} = a_1x_1(p_1 - x_1) + a_2x_2(p_1 - x_1) + e(p_1 - x_1) - r_1x_1$$

$$\frac{dx_2}{dt} = b_1x_1(p_2 - x_2) + b_2x_2(p_2 - x_2) + b_3y(p_2 - x_2) + e(p_2 - x_2) - r_2x_2$$

$$\frac{dy}{dt} = c_1x_2(q - y) + c_2z(q - y) + e(q - y) - r_3y$$

$$\frac{dz}{dt} = d_1y(r - z) + e(r - z) - r_4z.$$

The terms marked in red and blue are respectively the effects of blood transfusions and of deaths, which we will not consider yet, we thus assume $e = r_1 = r_2 = r_3 = r_4 = 0$. Here e is the infection rate from blood transfusions and r_i are the death rates for the different infected populations. The parameters we will focus on for now are: $a_1, a_2, b_1, b_2, b_3, c_1, c_2, d_1$, the infection rates between the different populations (due to sexual contact). We keep the rates of infection a_1 and a_2 between two males higher than the rates of hetero sexual contact (the other parameters), I assume, since the viral load in plasma (the liquid portion of blood) is higher than the viral load in semen [2]. Since anal penetration is more likely to result in tears than vaginal penetration [3], this supports the claim that homosexual sex between two males should have a higher infection rate than heterosexual sex. As a start I select the following values (as told by the assignment):

- $a_1 = 10$ and $a_2 = 5$

- $b_1 = 5$ and $b_2 = b_3 = 1$
- $c_1 = c_2 = 1$
- $d_1 = 1$

The populations should be scaled but as a start I use:

- $p_1 = p_2 = 5$
- $q = r = 100$

As initial conditions we assume that 1% of group (i) are infected and no one else:

$$x_1(t = t_0) = 0.01 \quad \text{and} \quad x_2(t = t_0) = y(t = t_0) = z(t = t_0) = 0$$

1.2 Solution

1.2.1 Forward Euler Method

One way of solving an initial value problem is the Forward Euler Method, which determines the initial slope y_0' of each component of the solution and using a step size h determines the next point from this by (p. 391 [1]):

$$y_1 = y_0 + hy_0' \tag{1}$$

This method is implemented in the code, through the function `forward_Euler`.

1.2.2 Fourth Order Runge Kutta Method

Runge Kutta methods are described in detail on p. 405 [1]. For this project we use the 4th order method, where the next step (from the initial/previous value) is found by:

$$y_{k+1} = y_k + \frac{h_k}{6}(k_1 + 2k_2 + 2k_3 + k_4) \tag{2}$$

where

$$k_1 = f(t_k, y_k) \tag{3}$$
$$k_2 = f(t_k + h_k/2, y_k + h_k \cdot k_1/2) \tag{4}$$
$$k_3 = f(t_k + h_k/2, y_k + h_k \cdot k_2/2) \tag{5}$$
$$k_4 = f(t_k + h_k, y_k + h_k k_3) \tag{6}$$

This method is implemented in the code, through the function `Runge_Kutta_4th`.

1.2.3 Implementation of Simulation

To simulate the spread of the HIV virus we first need to implement the differential equations given in the description. The equations are implemented on vector form in the function `diff_eq_HIV` in the attached python file. The function takes values of x_1, x_2, y and z at a given time step, stored in a single vector X along with the additional parameters in a list. It returns a vector `diff_X` which contains the values for $\frac{dx_1}{dt}$, $\frac{dx_2}{dt}$, $\frac{dy}{dt}$ and $\frac{dz}{dt}$. The function `simulate` uses one of the methods above to calculate each "next" time step and simulates the spread for N time steps of size dt.

1.2.4 Results for the Suggested Parameter Values

Using a small step size of $dt = 0.001$ both methods produce good results, which can be seen in the figure 1 below. The solutions look very similar although there is a larger discrepancy between the solutions for the heterosexual (dominant) population where the derivative is large and therefore harder to get right. One

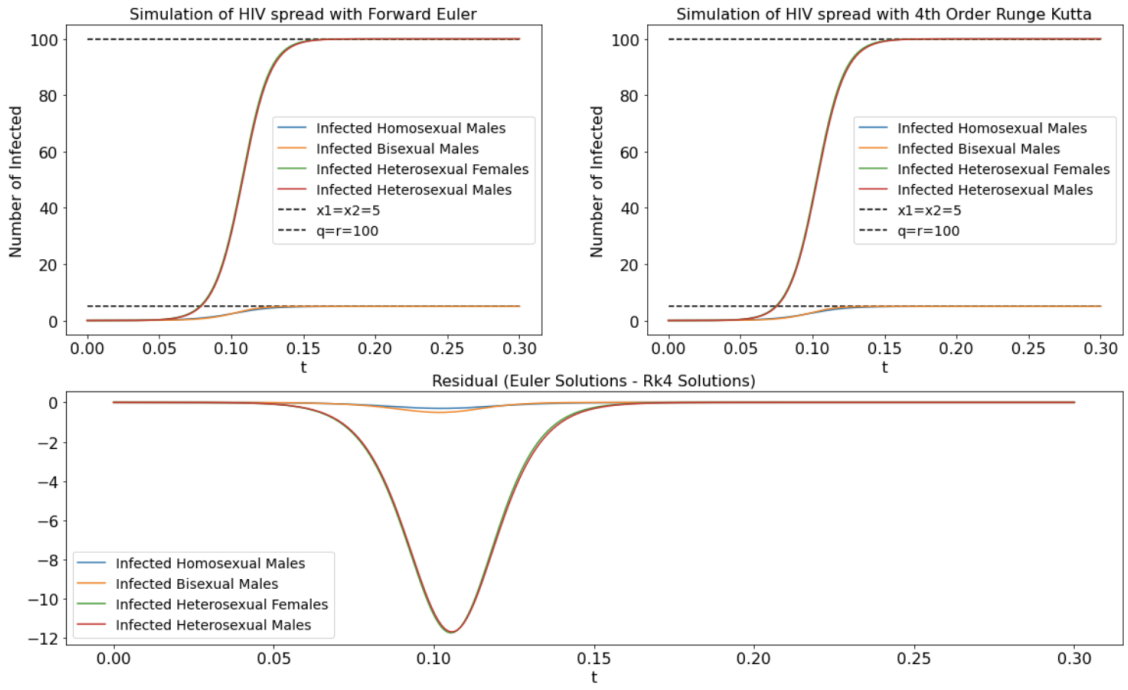

Figure 1: Simulation with dt=0.001 with the suggested parameter- and initial values from the assignment.

way we can examine the solution is by looking at the number of infected in each population at the end of the simulation. Since there are no death terms yet, no way to stop having sex (according to the equations) and viral suppression is not considered in the equations, we expect that by the end of the simulation everyone in all populations should be infected. This means that the number of infected in each population should be the size of the population. The numbers of infected by the end of simulations are reported for both methods in table 1 below. As is evident from the table, both methods are very precise for small step sizes such as $dt = 0.001$, although the forward Euler method comes slightly closer to the expected values. Another way to compare the two methods, is to see how quickly the solutions stabilize on a number

	Expected end values	End values from forward Euler method (dt=0.001)	End values from 4th order Runge Kutta Method (dt=0.001)
x_1	$p_1 = 5$	4.999999036594856	4.999998724725496
x_2	$p_2 = 5$	4.999999999988782	4.999999999966
y	$q = 100$	99.99999993639523	99.99999988679379
z	$r = 100$	99.99999982239561	99.99999970757855

Table 1: Number of infected in each population at the end of the simulations along with the expected values predicting all will be infected.

of infected for each population. To investigate this we define $\epsilon = 10^{-4}$ which denotes the criterion for which the number of infected may change between two consecutive points in our definition of stagnation. The function `t_stagnate` finds the time stamp where the criterion is upheld for all four populations and returns the average stagnation time of the four. It takes the input `t_cut` and only considers the solution after this time, since the solutions are "flat" in the beginning of the simulation when only 1% of p_1 are infected. For the forward Euler method we find that $t_{stagnate} = 0.2027$ and for 4th order Runge Kutta we find that $t_{stagnate} = 0.2022$. The Runge Kutta method thus finds the end value just a little quicker than the Euler method.

In general the two methods perform very similar for small step sizes. The advantage of the Runge Kutta

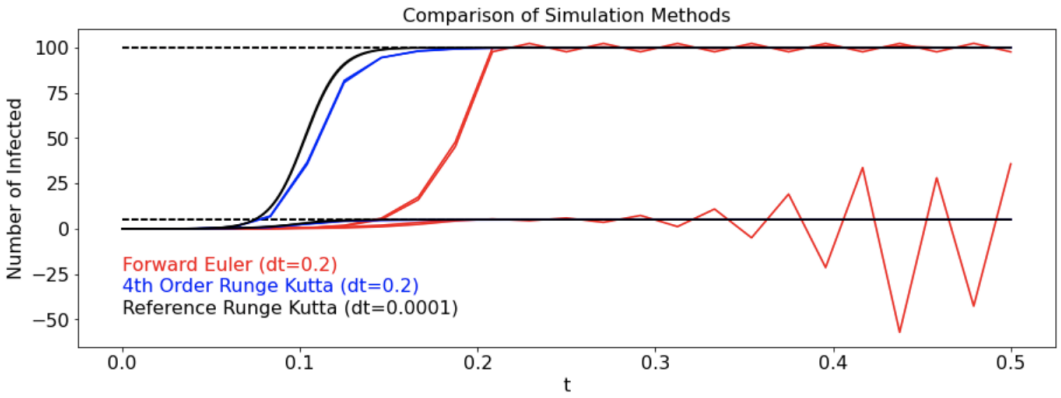

Figure 2: Comparing the performance of the two methods of simulating for a larger step size ($dt = 0.02$).

method is that it works for larger step sizes than the forward Euler method, and still performs okay when the forward Euler method breaks down and diverges. To illustrate this I performed the simulations again, now using a step size of 0.02 (20 times larger than before). To have a reference to compare the results to, the solutions are plottet along with the solution obtained from a $dt = 0.0001$ 4th order Runge Kutta simulation. This can be seen in figure 2 below. While the Runge Kutta method is less precise in the steepest part of the graph it does approach the right end values. In the forward Euler method people become infected much too late and the solution is not stable.

1.2.5 Exploring Different Parameters

When modelling the spread of HIV only through sexual contact there are three types of parameters we can change: population sizes, rates of infection and the initial values describing how many infected there are in each population in the beginning. In the code file all of these can be adjusted by changing `parameters` and `X0`, to explore the solutions I will only provide an example of change for each of the types of parameters.

Population Size

We keep the suggested values for infection rates and initial values, but change the size of each subpopulation so they all contain 100 individuals ($p_1 = p_2 = q = r = 100$). This implies that all the number of infected will stagnate at 100 for all populations, and allows us to more clearly see the effects of the suggested infection rates. The results from simulations with both methods are shown in figure 3 below. It is clear

that the slope of the number of infected homosexual males x_1 is the steepest, both since this is where we have placed the first infected individuals and since the infection rates included in this equation are the largest: $a_1 = 10$ and $a_2 = 5$. The slope of the number of infected bisexual males is almost as steep since these are in direct contact with the initially infected group, but a little less due to the lower infection rates: $b_1 = 5$, $b_2 = b_3 = 1$. The steepness of the slopes falls of for the remaining populations due to lower infection rates, and the last group to all be infected is the heterosexual males that are three degrees seperated from the homosexual males in terms of sexual contact.

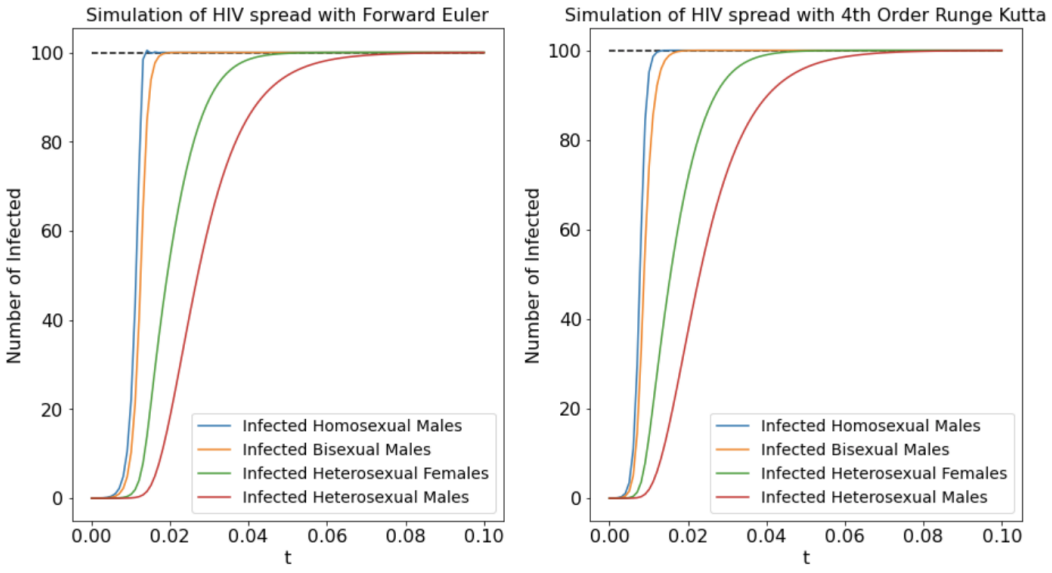

Figure 3: Simulation for population size of 100 for all subpopulations.

Rates of Infection

We keep the suggested values for population size and initial values, but change the infection rates so vaginal penetration (between a male and a female) has a higher infection rate than anal penetration (here assumed to be only between two males). In particular we let the infection rates be $a_1 = a_2 = b_1 = b_2 = 1$ and $b_3 = c_1 = c_2 = d_1 = 5$. The results from running a simulation with each method are displayed in figure 5 below. Here we see that even though the first infected individuals are in the homosexual male population, this population is the last to be fully infected, since they only have sexual contact with other males which we have assigned a lower infection rate. Heterosexual females and males experience the same infection rate during sexual contact, and thus become fully infected at the same time. The females are however one degree less seperated from the virus since only homosexual males are infected in the beginning, so if one zooms in quite a lot we can see they become fully infected just slightly before the heterosexual males.

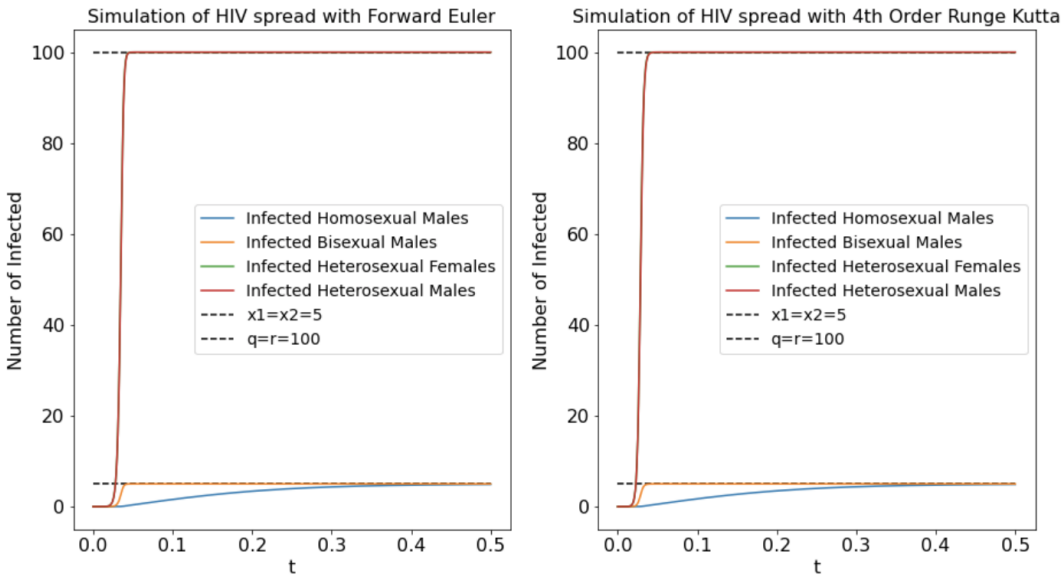

Figure 4: Simulation for infection rates of $a_1 = a_2 = b_1 = b_2 = 1$ and $b_3 = c_1 = c_2 = d_1 = 5$.

Initial Values

We keep the suggested values for population size and infection rates but change the initial values, i.e. which population contains infected individuals in the begining. Thus far we have seen that homosexual- and heterosexual males are the populations most separated from each other sexually, so we now let the first infected individuals be in the heterosexual male population to obtain the opposite direction of infection between the groups. We let $x_1 = x_2 = y = 0$ and $z = 0.01$. We observe that infection rates are more dominant than which population is the first to contain infected individuals, since despite the heterosexual males being the ones that introduce the desease to the entire group they are still the last to be fully infected. Different to what we observed when changing the population size we do, however, see that the bisexual males become fully infected before the homosexual males.

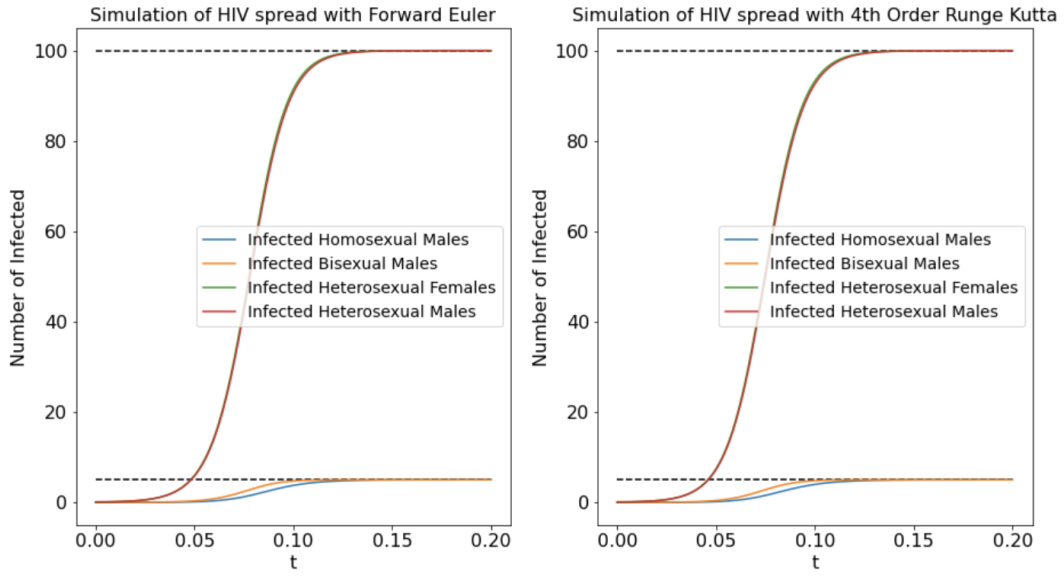

Figure 5: Simulation for initial values of $x_1 = x_2 = y = 0$ and $z = 0.01$.

2 Introducing the Effects of Blood Transfusion

To include the effects of blood transfusion we change the coefficient e from 0 (which excluded the effect) to $e = 0.001$ as suggested in the assignment. The results of the simulation performed with the two methods can be seen below in figure 6. Since the rate of infection from transfusion is so low compared to the sexual

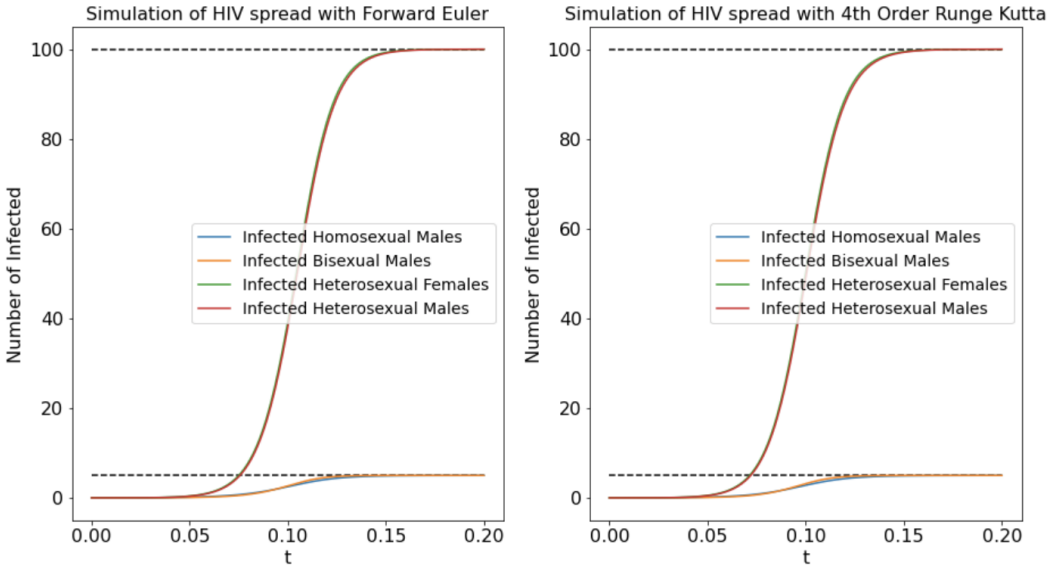

Figure 6: Simulation including blood transfusion with rate $e = 0.001$

infection rates and the term is constantly low, the effects are neglible. This attests to the fact that one is much less likely to get an infected blood transfusion than it is to have a sexual encounter with an infected individual. To better visualise the effect I increase the rate with a factor of a hundred to $e = 0.1$ and perform a 4th order Runge Kutta simulation and compare it to the previous result with the same method. This can be seen in figure 7 below. As expected the effect of adding infection from blood transfusion is that all individuals become infected faster.

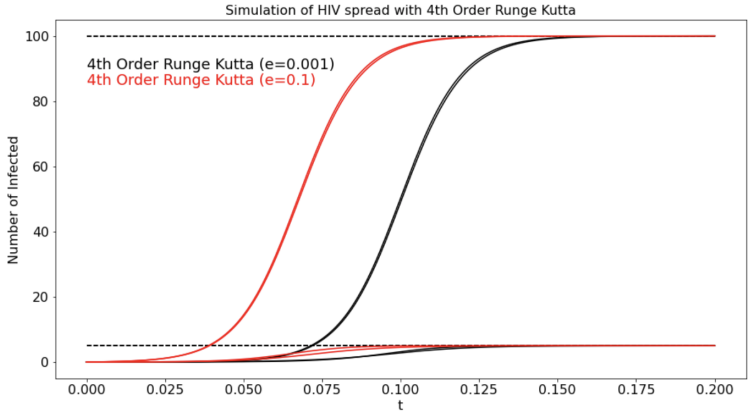

Figure 7: Comparing 4th order Runge Kutta simulations including blood transfusion with respectively $e = 0.001$ and $e = 0.1$

3 Introducing the Effects of Death

To include the effects of death we change the coefficients r_i from 0 (which excluded the effect) to $r_1 = r_2 = r_3 = r_4 = 0.05$. We continue to let $e = 0.001$ and keep the other suggested values from the assignment.The results of the simulation performed with the two methods can be seen below in figure 8. Again we don't see much change in the simulation, since the rate of death is much smaller than those of infection. To be able to see the effect we increase the death rates to $r_i = 10$ and obtain the results seen in

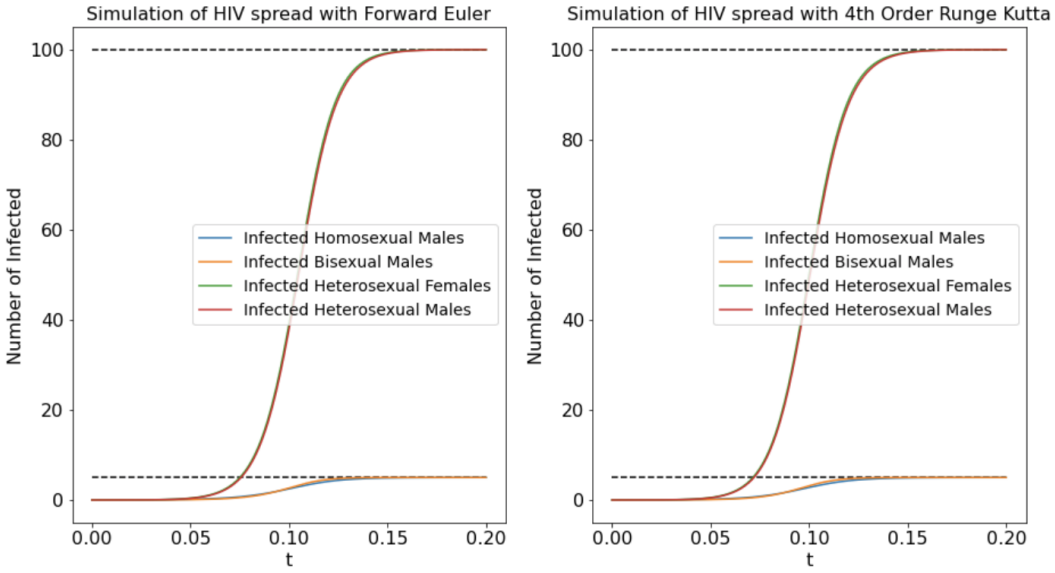

Figure 8: Simulation including death terms with rates $r_i = 0.05$

figure 9. As expected an increased death rate, reduces the total number of infected and the solutions stagnate at a lower number.

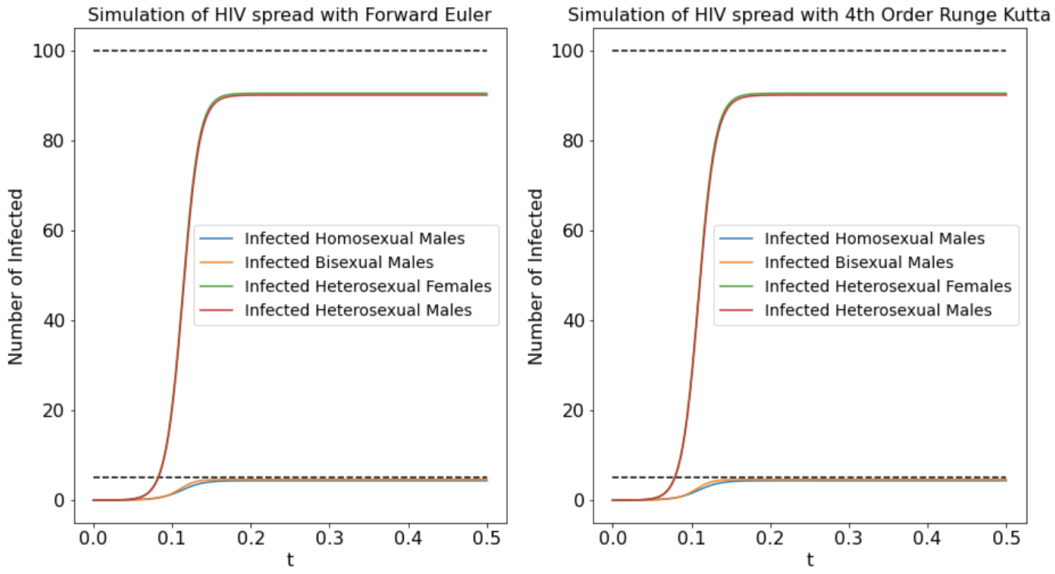

Figure 9: Simulation including death terms with rates $r_i = 0.10$

References

[1] Michael T. Heath, *Scientific Computing: An Introductory Survey*, 2nd Ed.

[2] Liuzzi G, Chirianni A, Clementi M, Bagnarelli P, Valenza A, Cataldo PT, Piazza M. Analysis of HIV-1 load in blood, semen and saliva: evidence for different viral compartments in a cross-sectional and longitudinal study. AIDS. 1996 Dec;10(14):F51-6. doi: 10.1097/00002030-199612000-00001. PMID: 8970677.

[3] Glick SN, Morris M, Foxman B, et al. A comparison of sexual behavior patterns among men who have sex with men and heterosexual men and women. J Acquir Immune Defic Syndr. 2012;60(1):83-90. doi:10.1097/QAI.0b013e318247925e