



Variable step length algorithms with high-order extrapolated non-standard finite difference schemes for a SEIR model



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ABSTRACT

In the present manuscript, higher-order methods are derived to solve a SEIR model for malware propagation. They are obtained using extrapolation techniques combined with nonstandard finite difference (NSFD) schemes used in Jansen and Twizell (2002). Thus, the new algorithms are more efficient computationally, and are dynamically consistent with the continuous model. Later, different procedures are considered to control the error in the discrete schemes. Numerical experiments are provided to illustrate the theory, and for the comparison of the different strategies in the adaptation of the variable step length.

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1. Introduction

Malware spreading is widely studied as it is a great threat to the information sharing. Furthermore, it represents one of the most serious security challenges we must face.

The spread of a malicious software, as occurs with a biological disease, involves not only the infectious agent (mode of transmission, latent period, susceptibility and resistance) [1], but in the case of malware, also the spatial structure [2], the device itself, and the environment where it could be disseminated, among others.

Most of the mathematical models proposed to study the dynamic transmission of malicious software are based on systems of ordinary differential equations (ODEs) from the epidemic theory [3]. The standard basic epidemic models are compartmental and consider separate sets for: susceptible (S) devices that could become infected; infected (I), who are able to transmit the malware; exposed (E), those in contact with malware but not yet infected; and recovered (R) that have gained immunity.

The acronyms for spreading models are based on the flow patterns between the compartments [4]. The SI model is the simplest one, as all the susceptible individuals or devices move to the infected compartment when they become infected, and remain in this compartment indefinitely. If these infected devices are recovered and come back to susceptible it is called SIS model, and if they die or acquire immunity to the malware then it is a SIR model [5].

Nevertheless, when the propagation of malware is studied, we have to take into account some specific characteristics that must be reflected in the equations that govern the dynamics of the model:

- (1) The communication networks are not static, they evolve over time considering the new devices that appear and the devices that disappear. As a consequence, some type of population dynamics has to be taken into account in the model.

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- (2) The new specimens of malware do not perform its malicious payload immediately after infection, but remain dormant during a certain period of time (this is one the characteristics of advanced persistent threats). Consequently it is necessary to include the exposed compartment in the model [6].
- (3) When the malware is successfully detected and removed (by using special security software), the device acquires permanent immunity due to the security patches installed. As a consequence, it is not usual to consider re-infection processes.

Thus, considering the above mentioned ideas, the more suitable model for its use in the study of malware propagation is the SEIR model:

$$\begin{aligned}
 \frac{dS}{dt} &= \mu(N - S) - \beta SI, & S(0) &= S_0, \\
 \frac{dE}{dt} &= \beta SI - (\mu + \sigma)E, & E(0) &= E_0, \\
 \frac{dI}{dt} &= \sigma E - (\mu + \gamma)I, & I(0) &= I_0,
 \end{aligned}
 \tag{1}$$

where $\mu, \beta, \sigma, \gamma$ are positive parameters, and the total population size, $N = S + E + I + R$, is constant over the time (thus $\frac{dR}{dt}$ can be written as combination of $\frac{dS}{dt}, \frac{dE}{dt}$ and $\frac{dI}{dt}$).

The SEIR epidemic model was approached from different perspectives. In [7,8] the global stability was analyzed when the term βSI of Eq. (1), known as incidence rate (the rate of new infections), is described by a nonlinear term. The global stability is also studied in [9,10], and [11], but in these cases for a non-varying population with different characteristics.

Some other methods were used for different SEIR models with specific considerations. For instance, the SEIR model with periodical repetitions of vaccinations against defined-age groups from a population was considered in [12], and the local asymptotic stability and the global asymptotic stability have been studied. The theory of the asymptotical autonomous differential systems, and the ideas of Li and Muldowney [8], have been used in [13] to reduce the four-dimensional SEIR model to a three-dimensional asymptotical autonomous differential system. In this case, authors considered an epidemic model in which the exposed and recovered individuals were infective. In [14], a system of differential equations with distributed infinite delay is considered, as the infectivity of the infected individuals varies according to a function of the age of infection.

In [15], authors applied the direct Lyapunov method, under the constant population size assumption, to prove that SEIR models, between others, display asymptotically stable steady states.

In this article, new schemes are derived to solve a SEIR model of malware dynamics. They will be obtained using extrapolation techniques combined with the first-order unconditionally stable nonstandard finite difference (NSFD) scheme proposed in [16]:

$$S^{n+1} = \frac{S^n + h_n \mu N}{1 + h_n(\mu + \beta I^n)}, \quad E^{n+1} = \frac{E^n + h_n \beta I^n S^{n+1}}{1 + h_n(\mu + \sigma)}, \quad I^{n+1} = \frac{I^n + h_n \sigma E^{n+1}}{1 + h_n(\mu + \gamma)}.
 \tag{2}$$

The fixed points of the proposed methods will be the same as the critical points of the SEIR model equations and they will have the same stability properties.

The idea of using Richardson’s extrapolation to obtain higher-order methods is well-known and it has been widely considered in the scientific literature (see [17,18], for example). First of all, we choose a numerical method of order p and compute the numerical results of the initial value problem (1) by performing n_i steps with step size h_i to obtain $y_{h_i}(x_0 + h) := T_{i,1}$. Afterwards we do these calculations for various values $h_1 > h_2 > h_3 > \dots$ (taking $h_i = h/n_i$, with n_i being a positive integer).

Then, the global error of any of these approximations has an asymptotic expansion of the form

$$y(x) - y_n(x) = e_p h^p + e_{p+1} h^{p+1} + \dots + e_N h^N + \dots.$$

The aim is to eliminate as many terms as possible from the asymptotic expansion above, by solving k linear equations for the unknowns y, e_p, \dots, e_{p+k-2} .

The outline of the paper is as follows. In Section 2, the numerical schemes are derived and it is demonstrated that they are dynamically consistent with the continuous model. Later, in Section 3, different procedures are considered to control the error in the discrete schemes. This is an important issue, since solutions can be considered stiff in some regions. Finally, in Section 4, some numerical tests are provided to compare different strategies in the adaptation of the variable step length.

2. Numerical schemes

2.1. Construction of the extrapolated nonstandard methods

Many sequences of integers n_i have been considered in Richardson’s extrapolation. In this manuscript, we are employing the so-called “harmonic sequence” (1, 2, 3, 4, 5, ...), which is considered a good election for polynomial extrapolation. However, it might be interesting to study (in the next future) some rational extrapolation as the “Bulirsch–Stoer” algorithm [19], for example.

Table 1
Stability properties of the continuous SEIR model (1).

β	Critical point	
	Trivial	Non-trivial
$< \beta^*$	Stable	Unstable
$= \beta^*$	Neutrally stable	–
$> \beta^*$	Unstable	Stable

Table 2
Convergence properties of the fixed points for the extrapolated nonstandard methods, considering that $h_n > 0, \forall n$.

Convergence	Critical point	
	Trivial	Non-trivial
Attracting	If $\beta \leq \beta^*$	If $\beta > \beta^*$
Repellant	If $\beta > \beta^*$	If $\beta \leq \beta^*$

In the case of the harmonic sequence, it is known that an easy way to calculate the $(k + 1)$ th method, $T_{j,k+1}$, is the Aitken–Neville algorithm:

$$T_{j,k+1} = T_{j,k} + \frac{(j - k)(T_{j,k} - T_{j-1,k})}{k}. \tag{3}$$

Now, we are able to obtain directly the second-order methods:

$$y(\widehat{x_0 + h}) = T_{2,2} = 2T_{2,1} - T_{1,1} = 2y_{h/2}(x_0 + h) - y_h(x_0 + h), \tag{4}$$

the third-order methods:

$$y(\widehat{x_0 + h}) = T_{3,3} = \frac{9y_{h/3}(x_0 + h) - 8y_{h/2}(x_0 + h) + y_h(x_0 + h)}{2}, \tag{5}$$

also fourth-order methods:

$$\begin{aligned} y(\widehat{x_0 + h}) &= T_{4,4} = \frac{-T_{1,1} + 24T_{2,1} - 81T_{3,1} + 64T_{4,1}}{6} \\ &= \frac{64y_{h/4}(x_0 + h) - 81y_{h/3}(x_0 + h) + 24y_{h/2}(x_0 + h) - y_h(x_0 + h)}{6} \end{aligned} \tag{6}$$

and so on.

2.2. Properties of the extrapolated NSFD schemes

The extrapolated schemes can be derived as $y(\widehat{x_0 + h}) = \sum_{i=1}^k c_i y_{h/i}(x_0 + h)$, and in all the cases with $\sum_{i=1}^k c_i = 1$, because $y(\widehat{x_0 + h})$ is always an approximation to $y(x_0 + h)$, hence $\sum_{i=1}^n c_i = 1$ is always the first equation we need to solve before eliminating the first terms from the asymptotic expansion. Now, we obtain the following theorem:

Theorem 1. *The new extrapolated nonstandard methods possess the stability properties that appear in Table 2, which are analogous to the stability properties of the continuous SEIR model. These stability properties of the continuous model are summarized in Table 1.*

The steady states of (1) with constant β are the standard ones [16] $S = N, E = 0, I = 0$, and the non-trivial critical points

$$S^* = \frac{(\mu + \sigma)(\mu + \gamma)}{\sigma \beta}, \quad E^* = \frac{\mu N}{\mu + \sigma} - \frac{\mu(\mu + \gamma)}{\sigma \beta}, \quad I^* = \frac{\mu \sigma N}{(\mu + \sigma)(\mu + \gamma)} - \frac{\mu}{\beta},$$

while the bifurcation point of the continuous model (1) is

$$\beta^* = \frac{(\mu + \sigma)(\mu + \gamma)}{\sigma N}.$$

Proof. It comes from the following two facts: (i) the original nonstandard finite difference method meets these convergence conditions (see [16]), and (ii) the extrapolated schemes were derived assuming that $y(\widehat{x_0 + h}) = \sum_{i=1}^k c_i y_{h/i}(x_0 + h)$, with $\sum_{i=1}^k c_i = 1$.

Now, let us suppose that $\lim_{t \rightarrow \infty} \lim_{h \rightarrow 0} y_h(x_0 + h) = \tilde{y}$, hence $\lim_{t \rightarrow \infty} \lim_{h \rightarrow 0} y_{h/i}(x_0 + h) = \tilde{y}$ and

$$\begin{aligned} \lim_{t \rightarrow \infty} \lim_{h \rightarrow 0} y(\widehat{x_0 + h}) &= \lim_{t \rightarrow \infty} \lim_{h \rightarrow 0} \sum_{i=1}^k c_i y_{h/i}(x_0 + h) \\ &= \sum_{i=1}^k c_i \lim_{t \rightarrow \infty} \lim_{h \rightarrow 0} y_{h/i}(x_0 + h) = \sum_{i=1}^k c_i \tilde{y}^{(ii)} = \tilde{y}, \end{aligned}$$

and therefore the new schemes converge at the same points and with the same conditions than their original nonstandard methods.

3. Variable-step algorithms

An adaptive step size selection is really important for an efficient integration of these models. Many procedures have been considered to control the error of ODEs including some described in [17,20].

For the methods proposed above, different techniques were considered including the following one [21,17]:

$$h_{n+1} = h_n \min(\text{facmax}, \max(\text{facmin}, \text{fac} \cdot (1/\text{err})^{1/k})), \tag{7}$$

with $\text{fac} = 0.5$, $\text{facmax} = 4$, $\text{facmin} = 10^{-1}$, and k is the order of the extrapolated method.

The value err describes how fast the length step increases or decreases. It is a quotient of the estimated error (calculated with $T_{k,k} - T_{k,k-1}$), and the tolerance (calculated with sc). The values for err and sc_i are calculated as usual:

$$\text{err} = \sqrt{\frac{1}{3} \sum_{i=1}^3 \left(\frac{(T_{k,k} - T_{k,k-1})_i}{sc_i} \right)^2}, \tag{8}$$

$$sc_i = ATol_i + \max(|y_{0,i}|, |T_{k,k,i}|) \cdot RTol_i, \tag{9}$$

where $y_{0,i}$ is the i th component of the solution at the previous step, and $T_{k,k,i}$ the i th component of the solution obtained through extrapolation.

It was also compared with a step size strategy with memory that was previously used by H.A. Watts [22], K. Gustafsson [23], and [24,25]:

$$h_{n+1} = h_n \min \left(\text{facmax}, \max \left(\text{facmin}, \text{fac} \cdot \frac{\text{err}_n^\alpha}{\text{err}_{n+1}^{1/k}} \right) \right), \tag{10}$$

where $\alpha = 0.08$ (when the previous step is accepted, if it is rejected $\alpha = 0$) as it was suggested in [23,17].

Different sets of parameters sc_i , $ATol_i$ and $RTol_i$ are considered and some comparisons will be provided in the numerical section, since this issue is very important for an efficient computation as it will be shown.

4. Numerical experiment

As in [16], we have considered the following parameter values:

$$\mu = 0.02, \quad \beta = 10^{-5}, \quad \gamma = 73, \quad \sigma = 45.6,$$

these parameters values correspond to a life expectancy of 50 years, an incubation period of 8 days (approximately) and an infectious period of, approximately, 5 days, respectively. Also, we took as initial values:

$$N = 5 \times 10^7, \quad s_0 = 125 \times 10^5, \quad e_0 = 5 \times 10^4, \quad i_0 = 3 \times 10^4.$$

In our experiments, the numerical methods converged to the correct fixed point (for large t_{end} values):

$$S^* = 7.305203 \times 10^6, \quad E^* = 1.871758 \times 10^6, \quad I^* = 1.168887 \times 10^4.$$

Standard methods do not always preserve the stated properties of these types of models. In general, this cannot be guaranteed or at least cannot be guaranteed for all step sizes. Some examples for similar autonomous systems can be found in [26–29] for example. Traditional Runge–Kutta methods do not guarantee the positivity of the solution and thus have problems of stability, and may require very small step length.

First of all, we computed the solutions at $t_{end} = 50$ with $h = 0.08, 0.04, 0.02$ and 0.1 for our schemes. But also for the standard Heun’s method, the trapezoidal (modified Euler also called improved Euler) and the most common fourth-order Runge–Kutta schemes (also called RK4). Heun’s method and the trapezoidal second-order Runge–Kutta schemes provided overflow values for $h = 0.08, 0.04$, and errors were very large for 0.02 and 0.1 . They converged rapidly for smaller values.

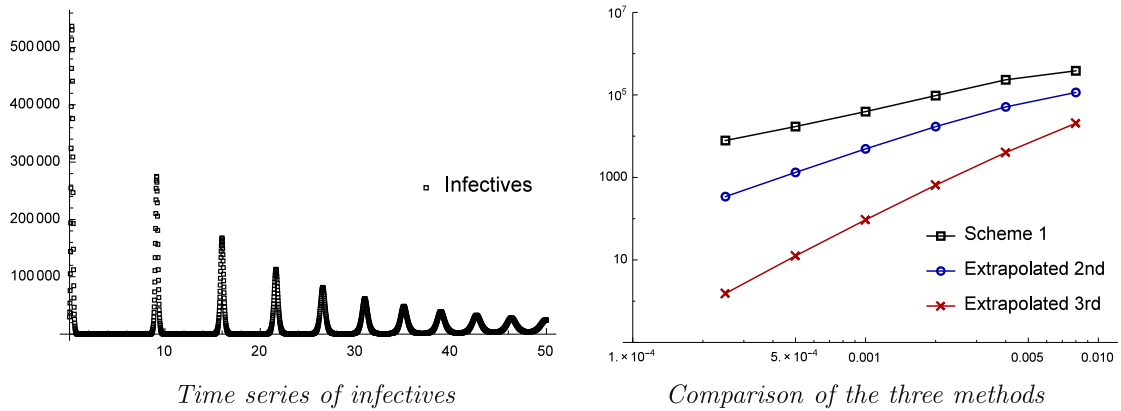


Fig. 1. Numerical simulations for infective devices/people i , obtained with the third-order scheme, in the interval $[0, 50]$ with $h = 10^{-4}$ (left side); and errors, in L_2 norm, with the non-standard scheme derived in [16], and its extrapolated second- and third-order variants (right side).

RK4 obtained NaN values for some h values under 10^{-3} . Our schemes were dynamically consistent with the continuous model.

Later, we also tested with some well-known variable step-length algorithms. We calculated the results in this problem with ode45 and ode23s. The first one is explicit and ode23s is implicit and usually considered for stiff problems. We did all the computations with the default parameters for both codes.

ode23s had many difficulties. It tried to utilize large length steps, but it got negative values for infectives at $t_{end} = 50$. This suggested us that ode23s might have more problems in a larger interval of integration. Hence, we tried to integrate until $t_{end} = 100$. However, Matlab gave an error: it was “Unable to meet integration tolerances without reducing the step size below the smallest value allowed”. It is clear that some values became negative and this totally changed the stability of the numerical schemes.

Surprisingly ode45 had a better behavior. It utilized much smaller length steps, specially near the origin. With the default values (for tolerance, ...), some of the values become negative near $t_{end} = 5$. These negative numbers look unrealistic. However, they are only $O(10^{-6})$, and ode45 is able to integrate until $t_{end} = 50$ or $t_{end} = 100$.

Now, we will focus our results in how accurate are the new extrapolated methods. Thus, we will study the errors again at $t_{end} = 50$. In Fig. 1 it is shown a numerical representation of the infectives produced by the extrapolated third-order scheme in the interval $[0, 50]$ with $h = 10^{-4}$, the approximation is provided for $t_i = 20ih$. Also, in the right hand figure, we show a comparative of the errors (obtained at $t_{end} = 50$) with the original first-order non-standard method [16], and the new second- and third-order schemes ($h = 0.008, 0.004, 0.002, 0.001, 0.0005, 0.00025$). It is clear that the new algorithms derived in this work are able to obtain more accurate approximations.

Although the third-order method is very efficient, and with $h = 10^{-4}$ errors are very small in general, however it is difficult to know “a priori” how small these errors are. For this purpose, we derived and analyzed the variable-step algorithms. In Fig. 2 it is shown a comparison of the two strategies explained above, in (7) and (10), with two different sets of the parameters, $ATol_i$ and $RTol_i$. In total four different procedures were tested for both, the second-order algorithm (left side of the figure) and also the third-order one (right side):

- Procedure 1: we used (7) with $ATol_i = 0$ and $RTol_i = Tol/N$, for $Tol = 10^4, 10^3, 10^2, 10^1$ with the second-order method, and $Tol = 10^3, 10^2, 10^1, 1$ with the third-one.
- Procedure 2: we used (7) with $RTol_i = 0$ and $ATol_i = Tol/N$, for $Tol = 10^6, 10^5, 10^4, 10^3$ with the second-order method, and $Tol = 10^3, 10^2, 10^1, 1$ with the third-one.
- Procedure 3: we used (10) with the same $ATol_i$ and $RTol_i$ values in Procedure 1.
- Procedure 4: we used (10) with the same $ATol_i$ and $RTol_i$ values in Procedure 2.

It is easy to check that near the points where the solution varies quickly (and the ODE can be considered stiff), errors can become large if the relative tolerance is not considered (when $RTol_i = 0$). Thus, procedures 1 and 3 are clearly much more computationally efficient and safer (errors are similar to the prescribed Tol values).

In Fig. 3 we compare the numerical results with the second- and third-order algorithms for procedures 1 and 3 (for $Tol = 10^3$), with the exact solution obtained with a very small length step. As it can be checked they respect the dynamics of the continuous system. Third-order schemes have a much smaller number of nodes (we did not print all of them in the figures), than second-order algorithms.

5. Conclusions

Higher-order methods are constructed to solve a SEIR model for malware propagation. They are built from a nonstandard finite difference scheme previously derived. Thus, the new algorithms are demonstrated to be dynamically consistent with the continuous model.

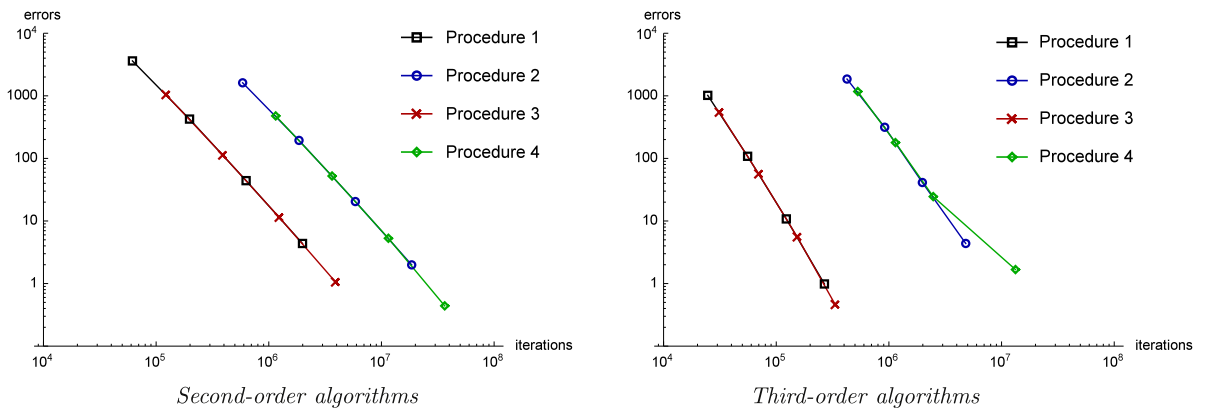


Fig. 2. Errors with four different procedures for second-order variable-step length algorithms (left side); and errors obtained with the third-order algorithms (right side). Errors are computed at $t_{end} = 50$ in L_2 norm.

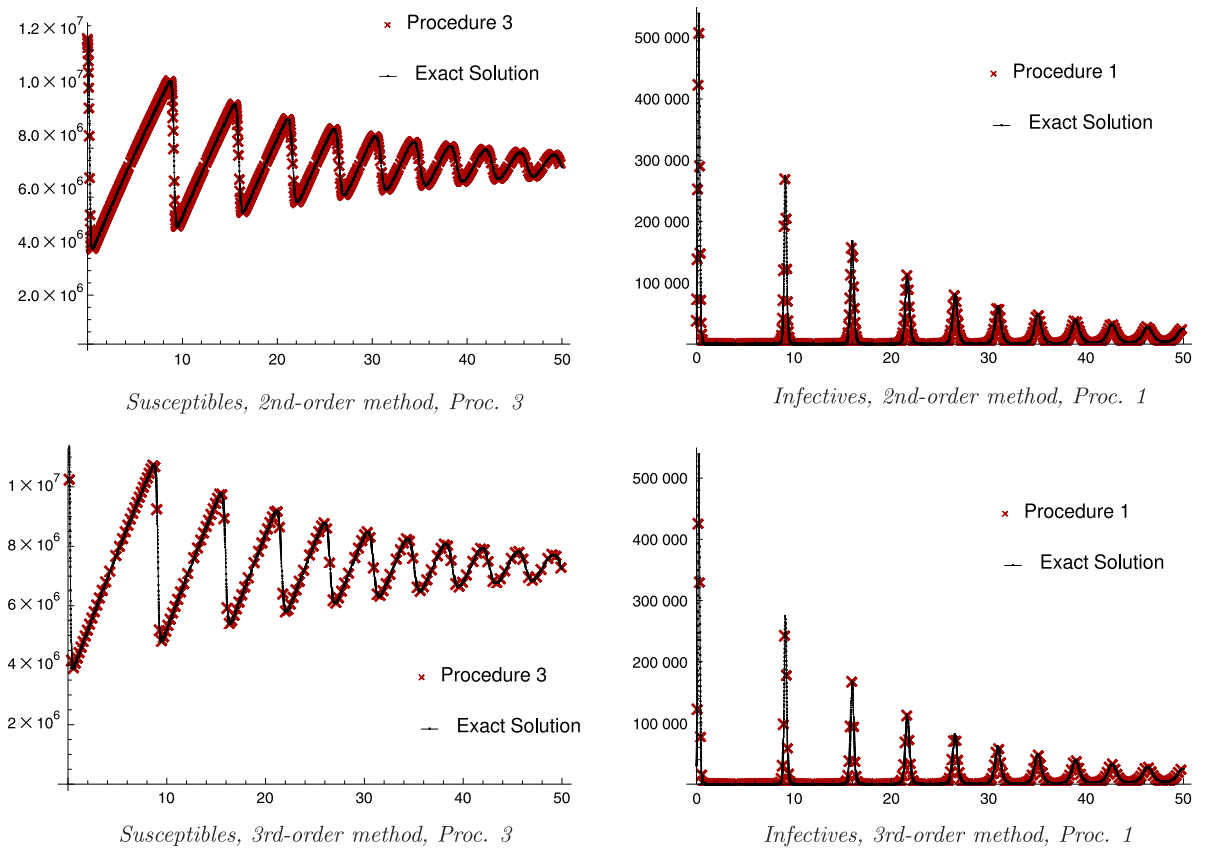


Fig. 3. Dynamics of susceptible and infective devices/people taken with the second- and third-order methods, with Procedures 1 and 3 and $Tol = 10^3$.

Numerical results show that solutions are very smooth in some regions, but in others, the model changes rapidly and some variables vary rapidly, hence it is necessary to address an adaptive step size selection. As far as we know, this is the first time that this issue has been studied in such type of models with a nonstandard finite difference scheme. Different procedures are proposed to control the error in the discrete schemes. Finally, these adaptive step size selections are compared and some numerical conclusions were provided.

The idea of combining extrapolated techniques together with other nonstandard finite difference schemes can be considered in the next future for other types of problems. They can provide higher-order methods with some desire properties for many other autonomous differential systems for which standard schemes have some difficulties.

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