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Topological structure preserving numerical simulations of dynamical models

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ABSTRACT

This paper brings together two methods producing numerical solutions with a statement of their quality — the nonstandard finite difference method and the method of validated computing. It deals with the construction and the analysis of reliable numerical discretizations of dynamical systems by employing these two techniques. An epidemiological model is used as a model example for their combined application.

1. Introduction

The systems of ordinary differential equations representing dynamical models in the natural sciences can seldom be solved explicitly. Typically a numerical procedure is applied for computing an approximate solution. In the standard numerical analysis, methods are investigated with regard to their convergence and rate of convergence. While the importance of convergence cannot be doubted it only makes a statement about the limit case when the parameters of the method approach some limit value (e.g. the step size h of a mesh going to zero) and only provided the computations are implemented exactly, i.e. there is no round-off error. Hence in practical simulations where an approximate solution is computed on a digital computer (with the corresponding rounding) for given values of the parameters of the method, e.g. some positive h, one needs a different kind of assurance about the quality of this solution. In this paper, which is partially based on the conference talk [1], we consider two approaches, both producing results with a statement of their quality, but addressing different aspects of the computed numerical solution. These are:

1. *The nonstandard finite difference method.* The aim of this method is numerical schemes preserving essential properties of the exact solution. In the case of dynamical systems these are properties like fixed points and their stability, periodic orbits, invariant sets, dissipativity, etc. The method relies on a novel way of constructing finite difference schemes by using renormalization of the denominator and nonlocal approximation of the nonlinear terms [2–4].
2. *Validated computing.* Computational round-off errors associated with real-number iterative methods prompted the development of self-verified methods utilizing interval analysis to calculate rigorous bounds of the solutions. The concepts of self-verified methods and their mathematical background are discussed in many works; see e.g. [5]. Mathematical rigor in the computer arithmetic using directed rounding, in algorithm design, and in program execution guarantees that the hypotheses of suitable inclusion theorems are (or are not) satisfied and thus guarantees that the stated problem has (or does not have) a solution in an enclosing interval. The extension to parameter-dependent problems led to self-verified solvers of parametric interval linear systems which provide guaranteed solution enclosures in floating-point computations [6,7].

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We discuss here the combined application of these two approaches to the construction and the analysis of numerical discretizations of continuous dynamical systems. A general setting of the problem is given in Section 2. The construction of numerical schemes uses an approach which is based on the concept of *topological dynamic consistency* [8,9], where the structural stability of maps plays an essential role. The discussion in Section 3 emphasizes the importance of selecting an appropriate space $\mathcal{V}$ for any given dynamical model so that the evolution maps $S(t)$ of the original system are $\mathcal{V}$ structurally stable. Then using a time mesh with a step size h we construct a numerical scheme with an evolution operator $F(h)$ such that $F(h) \in \mathcal{V}$ and it is also $\mathcal{V}$ structurally stable. For clarity of exposition we demonstrate the techniques on a concrete system, namely the SEIR($\rightarrow$S) epidemiological model presented in Section 4. Naturally, the area of application includes a much wider class of dynamical models in the applied sciences. A topologically dynamically consistent numerical scheme is constructed in Section 5 by using the nonstandard finite difference method. In Section 6 we discuss the applications of validated computations to (i) prove the numerical stability of the scheme; (ii) perform a rigorous componentwise sensitivity analysis of the model's response with respect to finite perturbations in the model parameters. The last section gives some concluding remarks.

2. General setting

Let W be an open subset of $\mathbb{R}^d$, $d \geq 1$. Consider the initial value problem

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

$$y(0) = x, \tag{2}$$

where $x \in W$ and $f \in C^0(W, W)$. We assume that (1) defines a (positive) dynamical system on $D \subset W$. This means that for every $x \in D$ the problem (1) and (2) has a unique solution $y = y(x, t) \in D$ for all $t \in [0, \infty)$. In a typical setting D is a compact subset of $\mathbb{R}^d$, but we do not need to make such an assumption upfront. For a given $t \in (0, \infty)$, the mapping $S(t) : D \to D$ given by $S(t)(x) \to y(x, t)$ is called the *evolution operator* and the set

$$\{S(t) : t \in (0, \infty)\} \tag{3}$$

is the well-known *evolution semigroup*. For every $x \in D$ the set $\{S(t)(x) : t \in (0, \infty)\}$ is called the (positive) orbit of x.

Suppose that the solution of (1) and (2) is approximated on the time grid $\{t_k = kh : k = 0, 1, \ldots\}$, where h is the time step, by a difference equation of the form

$$y_{k+1} = F(h)(y_k), \tag{4}$$

$$y_0 = x, \tag{5}$$

where the maps $F(h) : D \to D$ are defined for every $h > 0$. Hence, for every given $h > 0$, Eq. (4) defines a discrete dynamical system with an evolution semigroup $\{(F(h))^k : k = 1, 2, \ldots\}$. The orbit of a point $x \in D$ is the sequence $\{(F(h))^k(x) : k = 0, 1, 2, \ldots\}$.

The main aim of our investigation is the alignment of the properties of the systems (1)–(2) and (4)–(5). In this conceptual setting the structural stability of the evolution operators (3) of the original system and the evolution maps of its discretization, that is,

$$\{F(h) : h \in (0, \infty)\} \tag{6}$$

plays an important role. More precisely, in a typical setting of numerical analysis, a well posed problem is solved by a stable numerical method. This, in particular, means that small changes of the data change neither the solution of the original problem nor the approximate solution by the numerical method in significant ways. Therefore, looking at the problem and its discretization as dynamical systems one would require by analogy that small changes of the data do not affect in a significant way the properties of these dynamical systems. This, in essence, means that they both need to be structurally stable.

Definition 1. Let $\mathcal{V}$ be a topological space of maps from X to X. A map $f \in \mathcal{V}$ is called $\mathcal{V}$ structurally stable if there exists a neighborhood U of f in the topology of $\mathcal{V}$ such that every map $g \in U$ is topologically equivalent to f, that is, there exists a homeomorphism $\mu : X \to X$ such that

$$f \circ \mu = \mu \circ g. \tag{7}$$

In the general theory of topological dynamics the space $\mathcal{V}$ is typically $C^1(X, X)$. For models in practical applications this space is not always applicable. Hence the generalization given in Definition 1 is essential.

Structural stability for flows is defined in a similar way, where topological equivalency is replaced by orbit equivalency. It is important to note the different nature of the dynamical systems defined by (1) and (4). The first is a continuous dynamical system (a flow), while the second one is a discrete dynamical system. Most of the concepts of dynamical systems are defined for both continuous and discrete systems but very often, as is the case with structural stability as well, the meaning is different. In particular let us note that even if a flow is structurally stable, the maps $S(t_1)$ and $S(t_2)$ are not necessarily topologically equivalent when $t_1 \neq t_2$. To simplify matters and enhance the presentation of the main ideas, we replace the requirement that the flow defined by (1) is structurally stable with the stronger requirement that the maps $S(t)$, $t > 0$,

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are structurally stable. We should note that this assumption implies that there are no periodic orbits, thus limiting the dynamics of the system (1). Nevertheless, and as we show through examples, there are meaningful applications leading to such models. The reliability of the method (4) is in terms of correctly replicating the properties of the dynamical system that it approximates.

3. Topological dynamic consistency

The concept of topological dynamic consistency, introduced in [9], describes in precise terms the alignment of the properties of the discrete dynamical system and the approximated continuous dynamical system. We should remark that the issue of such alignment of properties has been approached in some parallel developments as well. For instance, the *geometric numerical integration* (see [10]) generally preserves first integrals of the system with the symplectic (area preserving) integration of Hamiltonian system being a well-known example. The *mimetic discretization* in [11] applies discrete equivalents of the physical laws yielding the continuous model. The approach in [9], which is extended here, is based on the important observation that the "dynamics" of dynamical systems, e.g. fixed points, periodic orbits, non-wandering sets, and the way these final states are approached, are topological properties. The similarity of a continuous dynamical system with the associated numerical methods, viewed as discrete dynamical systems, is in the sense of topological equivalence between the corresponding evolution operators.

Definition 2. The difference scheme (4) is called topologically dynamically consistent with the dynamical system (1) whenever all the maps in the set (3) are topologically equivalent to each other and every map in the set (6) is topologically equivalent to them. (Thus, the maps $S(t)$ and $F(h)$ are topologically the same for every $t > 0$ and $h > 0$.)

The next theorem provides a straightforward way of proving topological dynamic consistency via the structural stability of the evolution operators of the original system and its numerical method.

Theorem 3. *Let $\mathcal{V}$ be a topological space of maps from D to D such that it contains the sets (3) and (6) and the mappings $S : (0, \infty) \to \mathcal{V}$ and $F : (0, \infty) \to \mathcal{V}$ are both continuous. Let also the following conditions hold:*

(i) *for each $t > 0$ the map $S(t)$ is $\mathcal{V}$ structurally stable;*
(ii) *for each $h > 0$ the map $F(h)$ is $\mathcal{V}$ structurally stable;*
(iii) *there exists $h > 0$ such that $S(h)$ and $F(h)$ are topologically equivalent.*

Then the numerical method (4) is topologically dynamically consistent with the dynamical system (1).

Proof. The topological equivalence of maps is an equivalence relation in the space $\mathcal{V}$. Thus, we need to prove that maps in the two sets (3) and (6) belong to the same equivalence class. Let us see first that condition (i) implies that the maps $S(t)$, $t > 0$, are all topologically equivalent. Let $0 < t_1 < t_2$. From the structural stability of the maps $S(t)$, $t > 0$, it follows that for every $t \in [t_1, t_2]$ there exists a neighborhood W_t of $S(t)$ in $\mathcal{V}$ such that $S(t) \sim g$ for every $g \in W_t$. Since the map $S : (0, \infty) \to \mathcal{V}$ is continuous, for every $t \in (0, \infty)$ there exists δ_t such that $S(\tau) \in W_t$ whenever $|\tau - t| < \delta_t$. Then $\bigcup_{t\in[t_1,t_2]}(t - \delta_t, t + \delta_t)$ is an open cover of $[t_1, t_2]$. By the compactness of $[t_1, t_2]$ it follows that there exists a finite set $\{\tau_1, \tau_2, \ldots, \tau_k\}$ such that

$$[t_1, t_2] \subset \bigcup_{i=1}^{k}(\tau_i - \delta_{t_i}, t + \delta_{t_i}).$$

Without loss of generality we may assume that $\tau_1 = t_1$, $\tau_k = t_2$ and that the set is arranged in increasing order, that is, $\tau_i < \tau_{i+1}$. For an arbitrary pair τ_i, $\tau_i + 1$ there exists $\tau_{i+\frac{1}{2}}$ such that $\tau_{i+\frac{1}{2}} \in (\tau_i - \delta_{\tau_i}, \tau + \delta_{\tau_i}) \cap (\tau_{i+1} - \delta_{\tau_{i+1}}, t_{i+1} + \delta_{\tau_{i+1}})$. Therefore $S(\tau_{i+\frac{1}{2}}) \in W_{\tau_i} \cap W_{\tau_{i+1}}$, which implies that $S_{\tau_i} \sim S_{\tau_{i+1}}$. Then using induction we obtain that $S_{\tau_1} \sim S_{\tau_k}$ or equivalently $S_{t_1} \sim S_{t_2}$. Hence all maps $S(t)$, $t > 0$, are topologically equivalent to each other.

Using a similar argument we obtain from condition (ii) that all maps $F(h)$, $h > 0$, are topologically equivalent to each other. The statement of the theorem then follows from (iii). □

Remark 4. Properties (i) and (ii) in Theorem 3 are attributes of the problem and the method respectively. Property (iii) provides a link between the problem and the method which may be considered an analogue of the consistency of the scheme since the value of h in (iii) is typically unknown and is described as sufficiently small. This property is established for a variety of numerical methods in the work of M.-C. Li (see [12,13]), following earlier work of B.M. Garay (see [14,15]). In all cases the topological equivalence is established for sufficiently small h. We should emphasize the fact that Theorem 3 provides topological equivalence of the respective evolution operators for all values of h and t, thus implying the topological dynamic consistency of the scheme.

The main ingredient in Theorem 3 is the structural stability of the maps involved. Deriving sufficient conditions for structural stability of flows and diffeomorphisms is one of the greatest achievements of topological dynamics with main contributions from Anosov, Moser, Palis, Smale, Robin and Robinson [16]. The current form of the structural stability theorem, proved in [17,18], states that flows and diffeomorphisms on a compact manifold without boundary which satisfy Axiom A and the strong transversality condition are structurally stable. In particular, Morse–Smale flows and

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diffeomorphisms on a compact manifold are structurally stable; see [19, Theorem 12.2]. In all these theorems the structural stability is considered with respect to the space $C^1(X, X)$. Hence, and as mentioned in the general setting above, their practical application could be rather limited. For example, the evolution operator of the epidemiological model considered in the next section is not C^1 structurally stable since it has an invariant set on the boundary and a fixed point which is not necessarily hyperbolic. Our approach in such cases is to design for the given model an appropriate space $\mathcal{V}$ so that the respective evolution operator is structurally stable. Then we construct a discretization such that the evolution operator of the numerical scheme is in $\mathcal{V}$ and is also $\mathcal{V}$ structurally stable. Then the topological dynamic consistency of the scheme follows from Theorem 3.

4. SEIR(→ S) model

As a model example for the application of the theory derived so far we consider a basic compartmental model for the spread of an infectious disease in a given population. The course of the disease is schematically represented as

$$S \longrightarrow E \longrightarrow I \longrightarrow R\ (\longrightarrow S),$$

where S denotes the number of susceptible individuals, E the number of exposed individuals (carriers which are not yet infective), I the number of infectives and R the number of recovered individuals with immunity. The following mathematical model is derived in [20, Chapter 21] as a system of differential equations for the fractions of the respective classes in the total population N, that is, $u = \frac{S}{N}, x = \frac{E}{N}, y = \frac{I}{N}, u = \frac{R}{N}$:

$$\begin{cases} \dfrac{du}{dt} = \nu(1-u) - uy + \eta z \\ \dfrac{dx}{dt} = uy - (\xi + \nu)x \\ \dfrac{dy}{dt} = \xi x - (\theta + \nu)y \\ \dfrac{dz}{dt} = \theta y - (\eta + \nu)z. \end{cases} \tag{8}$$

The time is scaled in a such a way that the coefficient of the nonlinear term uy representing the mass action principle for the spread of the infection equals 1. The nonnegative constants ξ, θ and η model the rates of transfer between the respective compartments, while ν is linked to the life expectancy under the assumption of constant population.

The system of ODEs (8) defines a dynamical system on the three-dimensional simplex

$$G = \{(u, x, y, z) : u \geq 0, x \geq 0, y \geq 0, z \geq 0, u + x + y + z = 1\}. \tag{9}$$

Hence, one can eliminate one of the variables, e.g. u, and obtain the system in the following equivalent form:

$$\begin{cases} \dfrac{dx}{dt} = (1 - x - y - z)y - (\xi + \nu)x \\ \dfrac{dy}{dt} = \xi x - (\theta + \nu)y \\ \dfrac{dz}{dt} = \theta y - (\eta + \nu)z \end{cases} \tag{10}$$

where (10) defines a dynamical system on the compact domain

$$D = \{(x, y, z) : x \geq 0,\ y \geq 0,\ z \geq 0,\ x + y + z \leq 1\}.$$

The point (0, 0, 0) is always an equilibrium of (10). This is the Disease Free Equilibrium (DFE). The system may have another equilibrium, namely,

$$z_e = \frac{\theta\nu(\mathcal{R}_0 - 1)}{\nu + \eta - \eta\theta\mathcal{R}_0}, \qquad y_e = \frac{\nu + \eta}{\theta} z_e, \qquad x_e = \frac{\nu + \theta}{\xi} y_e, \tag{11}$$

where $\mathcal{R}_0 = \frac{\xi}{(\nu+\xi)(\nu+\theta)}$ is the basic replacement ratio. The point in (11) is an equilibrium of the dynamical system (10) whenever it belongs to its domain D, that is, whenever $\mathcal{R}_0 > 1$. It is called an Endemic Equilibrium (EE) since it describes a permanent presence of the disease. Our concerns here are the properties of the dynamical system (10). It was proved in [20, Theorem 21.2] that:

- If $\mathcal{R}_0 \leq 1$ then DFE is globally asymptotically stable on D. (12)
- If $\mathcal{R}_0 > 1$ then DFE is a hyperbolic saddle point with stable manifold
  $\Gamma = \{(x, y, z) \in D : x = y = 0\}$, and EE is stable and attracting with basin of attraction $D \setminus \Gamma$. (13)

It is easy to see that the maps $S(t)$ for the dynamical system (10) are not C^1 structurally stable due to the fact that they have a fixed point and an orbit on the boundary of the domain D. In order to obtain structural stability for $S(t)$ we consider the

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following smaller space:

$$\mathcal{V} = \left\{ g : D \to D : \begin{vmatrix} (1)\, g : D \to g(D) \text{ is a diffeomorphism} \\ (2) \text{ DFE is a fixed point of } g \\ (3)\ \Gamma \text{ is invariant and in the stable manifold of DFE} \end{vmatrix} \right\}.$$

Note that all the maps in $\mathcal{V}$ have the "unstable" features of $S(t)$, which leads to the following theorem.

Theorem 5. *For every $t > 0$ the evolution operator $S(t)$ is $\mathcal{V}$ structurally stable provided*

$$(\nu + \xi + \theta)(\nu + \eta) > \theta\xi. \tag{14}$$

The proof is carried out by essentially the same method as the proof of [21, Theorem 16.3.1], where the structural stability of flows with a single globally attractive fixed point is established. Condition (14) ensures that whenever DFE is $\in D \setminus \Gamma$, its basin of attraction is $D \setminus \Gamma$; see [20, Theorem 21.11]. Hence it can be replaced by any other condition implying the said property, e.g. $\eta = 0$; see [20, Theorem 21.12].

5. A $\mathcal{V}$-structurally stable scheme based on the nonstandard finite difference method

Traditionally the main concerns of numerical analysis are the stability, convergence and rate of convergence of numerical methods. While the importance of convergence is not in doubt, it often happens that essential properties of the approximated models are lost in the discretization of the differential equations. These may include the physical laws (e.g. conservation of mass, energy or momentum) used to construct the differential models. The main contribution of the nonstandard finite difference method to the field of numerical analysis is the conceptual base and the tools for preserving essential physical properties of the models, [22,2–4]. There has been a considerable effort in recent years to construct numerical procedures which correctly replicate the properties of the original dynamical system by using the nonstandard finite difference method. In fact the concept of *dynamic consistency*, which was made precise in the recent works of the author and his collaborators, originally appeared in the context of this method [23,2,3]. The following scheme, which uses nonlocal approximation of the nonlinear term similarly to [24], is crafted in such a way that the operator $F(h)$ is in $\mathcal{V}$ and it is also $\mathcal{V}$ structurally stable:

$$\begin{cases} \dfrac{u_{k+1} - u_k}{h} = -u_{k+1}y_k + \nu x_{k+1} + \nu y_{k+1} + (\eta + \nu)z_{k+1} \\ \dfrac{x_{k+1} - x_k}{h} = u_{k+1}y_k - (\xi + \nu)x_{k+1} \\ \dfrac{y_{k+1} - y^n}{h} = \xi x_{k+1} - (\theta + \nu)y_{k+1} \\ \dfrac{z_{k+1} - z^n}{h} = \theta y_{k+1} - (\eta + \nu)z_{k+1}. \end{cases} \tag{15}$$

Let us note that we discretize the four-equation form (8) of the dynamical system since then the method is more convenient for both implementation and theoretical analysis. This does not increase the computational complexity since the values of u_{k+1} need to be calculated anyway. The method is implicit but any time step involves only the solution of a linear system

$$C(h, y_k) \begin{pmatrix} u_{k+1} \\ x_{k+1} \\ y_{k+1} \\ z_{k+1} \end{pmatrix} = \begin{pmatrix} u_k \\ x_k \\ y_k \\ z_k \end{pmatrix}, \tag{16}$$

where

$$C(h, y_k) = \begin{pmatrix} 1 + hy_k & -h\nu & -h\nu & -h(\eta + \nu) \\ -hy_k & 1 + h(\xi + \nu) & 0 & 0 \\ 0 & -h\xi & 1 + h(\theta + \nu) & 0 \\ 0 & 0 & -h\theta & 1 + h(\eta + \nu) \end{pmatrix}.$$

Preserving the conservation law in the definition of G in (9), as for all population models (see [25]), is of fundamental importance. From the formulation (16) it is easy to see that starting from an initial condition in G we have

$$u_{k+1} + x_{k+1} + y_{k+1} + z_{k+1} = u_k + x_k + y_k + z_k = 1. \tag{17}$$

Further, since the matrix $C(h, y_k)$ is a strictly column diagonally dominant M-matrix, its inverse is nonnegative. Hence the nonstandard scheme (15), in addition to satisfying the conservation law (17), also preserves the nonnegativity of the vectors. Therefore, it defines a discrete dynamical system on G.

Eq. (17) also shows that (u_k) can be eliminated in exactly the same way as u is eliminated in (8). The reduced linear system

$$\hat{C}(h, y_k) \begin{pmatrix} x_{k+1} \\ y_{k+1} \\ z_{k+1} \end{pmatrix} = \begin{pmatrix} x_k \\ y_k \\ z_k \end{pmatrix}, \tag{18}$$

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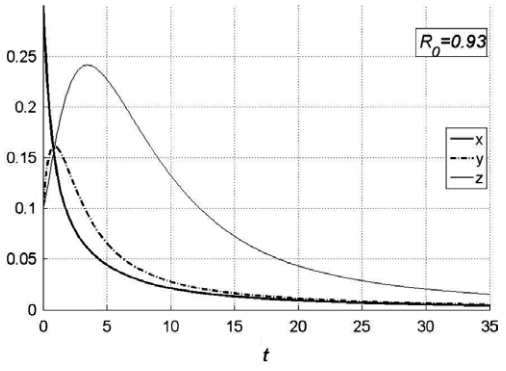

Fig. 1.

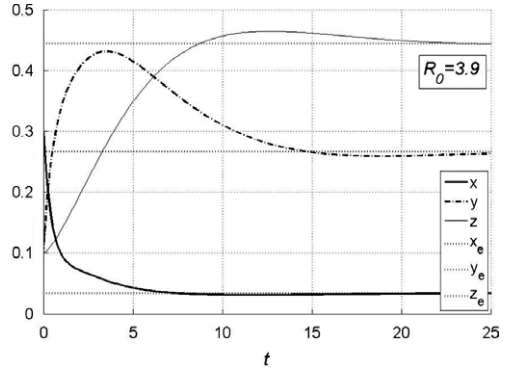

Fig. 2.

where

$$\hat{C}(h, y_k) = \begin{pmatrix} 1+h(\xi+\nu) & 0 & 0 \\ -h\xi & 1+h(\theta+\nu) & 0 \\ 0 & -h\theta & 1+h(\eta+\nu) \end{pmatrix}$$

represents a discretization of (10) and defines a discrete dynamical system on D. The evolution map $F(h) : D \to D$ (see (4)) for the scheme (18) is given by

$$F(h)\begin{pmatrix} x \\ y \\ z \end{pmatrix} = C(h, y)\begin{pmatrix} x \\ y \\ z \end{pmatrix}. \tag{19}$$

Now it is easy to see that $F(h)$ is a diffeomorphism and that DFE is an equilibrium of $F(h)$ with stability properties as described in the definition of $\mathcal{V}$. Therefore, $F(h) \in \mathcal{V}$. Moreover using an argument similar to that in the proof of Theorem 5 we obtain the following theorem.

Theorem 6. *For every $h > 0$ the evolution map $F(h)$ given in (19) is $\mathcal{V}$ structurally stable provided (14) holds.*

The approximate solutions for two sets of constants are presented in Figs. 1 and 2. In Fig. 1 we have $\mathcal{R}_0 = 0.93 < 1$ while $\mathcal{R}_0 = 3.9 > 1$ in Fig. 2 and one may observe that the properties of the exact solutions in (12) and (13) are correctly replicated. We note that it may happen that standard methods also preserve the stated properties. However, in general, this cannot be guaranteed or at least cannot be guaranteed for all step sizes. Examples to that effect for similar systems can be found in [8,9]. See also [4,22,2,3] for a general discussion on the issue.

6. Sensitivity analysis via validated computing

Structural stability does not imply numerical stability. Therefore we apply advanced methods for bounding the solution of a linear system involving interval parameters [6,7]

(i) to demonstrate quantitatively the numerical stability of the iteration scheme (16), and
(ii) to perform a rigorous componentwise sensitivity analysis with respect to finite perturbations in the model parameters.

The computations are done separately for the two sets of constants considered at the end of previous section and presented in Table 1.

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Table 1
Nominal values for the SEIR model parameters illustrating DFE (12) and EE (13) properties.

Model property	ν	ξ	θ	η	$\mathcal{R}_0$
DFE	0.2	1	0.7	0.07	0.926
EE	0.05	2	0.2	0.1	3.9

Table 2
Maximum relative diameters of the intervals enclosing the solution.

Model property	1st iteration	351st iteration
DFE	5.3×10^{-15}	2.6×10^{-11}
EE	5.1×10^{-15}	1.0×10^{-10}

Table 3
Componentwise sensitivity ($10f$) for $\mathcal{R}_0 < 1$.

Solution component	ν	ξ	θ	η	All parameters
x	3.57	6.33	4.06	0.91	7.56
y	3.89	6.92	4.45	0.98	8.23
z	9.42	16.57	10.08	2.38	19.9

Table 4
Componentwise sensitivity (f) for $\mathcal{R}_0 > 1$.

Solution component	ν	ξ	θ	η	All parameters
x	8.26	30	14	5.67	32
y	40.94	149	72	29	159
z	27.00	98	47	19	105

First, we run the iteration scheme solving at each step a linear system (16) with guaranteed bounds for the solution components $(u_k, x_k, y_k, z_k) \in ([u_k], [x_k], [y_k], [z_k])$. Since the coefficient matrix $C(h, y_k)$ of (16) depends on y_k, we apply self-verified methods for solving parametric linear systems [7]. The model parameters are considered having their nominal values. Thus, at the first iteration step the maximal relative diameter of the intervals bounding the solution components is about 5.3×10^{-15} for both numerical experiments; see Table 2. The intervals bounding the solution get into the system at the next iteration step and thus propagate the round-off errors. This is the so-called wrapping effect in interval computations which blows up the interval box enclosing the solution at each iteration. Nevertheless, the numerical stability of the iteration scheme is demonstrated. The maximal relative diameter at the last (351st) iteration step is 2.6×10^{-11} in the DFE case and one order of magnitude greater, 1.0×10^{-10}, in the EE case; see Table 2.

Next we estimate the sensitivity of the linear system (16) with respect to perturbations in the model parameters ν, ξ, θ, η. It is shown in [26] that traditional condition numbers do not necessarily reflect the true sensitivity of the solution components. While a single condition number is given by the classical sensitivity analysis, we perform a componentwise sensitivity analysis of the solution.

Let a linear system $A(p)x = b(p)$ depending on an m-tuple of parameters $p = (p_1, \ldots, p_m)$ be given, with $A(p)$ invertible. For parameters varying within given tolerances $p \in [p] \in \mathbb{IR}^m$, $[p] = p(1 \pm \varepsilon)$ and small $\varepsilon > 0$, the diameter of the solution set $\Sigma(A(p), b(p), [p]) := \{A^{-1}(p)b(p) \mid p \in [p]\}$ gives a componentwise measure of the sensitivity of the solution $A^{-1}(p)b(p)$ w.r.t. small changes in the parameters p. For $[s] \in \mathbb{IR}^n$, $[s] \supseteq \Sigma(A(p), b(p), [p])$,

$$f := \operatorname{diam}([s])/(2\varepsilon) \geq \operatorname{diam}(\Sigma(A(p), b(p), [p]))/(2\varepsilon)$$

bounds the maximum factor by which an ε-perturbation of the parameters p is amplified in terms of variations in the solution.

In the following we present the componentwise sensitivity analysis performed separately for each linear system corresponding to the two model properties, namely the parameter values given in Table 1. The sensitivity was estimated separately with respect to each model parameter and w.r.t. all model parameters altogether. The iteration scheme was run solving at each step the corresponding system (16) with $\varepsilon = 10^{-12}$ for the corresponding perturbed model parameter(s). Tables 3 and 4 display f for the solution components at the last iteration step. Due to an automatic error control mechanism the accuracy of every computed result is guaranteed.

As can be seen from Tables 3 and 4, the overall sensitivity of the two systems corresponding to the two model properties is small, although the system representing the EE property ($\mathcal{R}_0 > 1$) has two orders of magnitude greater sensitivity than the system representing the DFE property. It is demonstrated that some individual solution components are much more responsive to perturbations in the input parameters than others.

In both cases, Tables 3 and 4, the variations in the parameter η influence the system solution less, while the parameter ξ is most responsible for the variations in the solution. The componentwise sensitivity obtained clearly demonstrates the

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difference between the two model properties. Namely, the contribution of a given parameter to the variations in the solution components differs between the two model systems. For example, the y solution component is most variable in the case of the EE property, while in the case of the DFE property the most variable solution component is z.

An analysis of the componentwise sensitivity of a system with respect to the parameters involved is of particular importance when studying models involving unknown but bounded model parameters.

7. Conclusion

The paper deals with reliable numerical discretizations of continuous dynamical systems arising as models for different natural phenomena, with a focus on schemes which correctly replicate the properties of the original dynamical systems. The construction and the analysis of such schemes is based on two techniques: the nonstandard finite difference method and the method of validated computing. Their combined application is demonstrated on an epidemiological model. These two approaches can be linked in applications in more than one way and future research will seek such applications to models of practical significance.

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