Reliable Simulations for Applied Dynamical Models[1]

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Abstract. The paper deals with the construction and the analysis of reliable numerical discretizations of dynamical systems by employing two different techniques: the nonstandard finite difference method and the method of validated computing. An epidemiological model is used as a model example for the application of these techniques.

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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 roundoff error. Hence in practical simulations where an approximate solution is computed on a digital computer (with respective 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 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, [5].
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. [9]. Mathematical rigor in the computer arithmetic using directed rounding, in algorithm design, and in program execution guarantee that the hypotheses of suitable inclusion theorems are (or are not) satisfied and thus guarantee 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 [7, 8].

We discuss here the combined application of these two approaches to the construction and the analysis of numerical discretizations of continuous dynamical systems. For clarity of the exposition we demonstrate the techniques on a concrete system, namely the SEIR($\rightarrow$S) epidemiological model presented in Section 2. Naturally, the area of application includes a much wider class of dynamical systems. The nonstandard scheme discussed in Section 3 is derived by using structural stability of maps. Let us recall that, given a topological space X and a topological space $\mathscr{V}$ of maps from X to X, a map $f \in \mathscr{V}$ is called *$\mathscr{V}$ structurally stable* if there exists a neighborhood U of f in the topology

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of $\mathscr{V}$ such that every map $g \in U$ is topologically equivalent to f, that is, there exists a homeomorphism $\mu : X \to X$ such that $f \circ \mu = \mu \circ g$. Let us note that in the general theory of topological dynamics the space $\mathscr{V}$ is typically $C^1(X,X)$. In particular the well known structural stability theorems are also in such setting with X being a compact manifold without boundary. These theorems treat essentially idealized situations not necessarily common in applied models like the epidemiological model discussed in the next section. The discussion in Section 3 emphasizes the importance of selecting an appropriate space $\mathscr{V}$ for any given dynamical model. For the construction of the numerical scheme we follow the approach in [1]. First we define a space $\mathscr{V}$ such that the evolution maps $S(t)$ of the original system are $\mathscr{V}$ 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 $F(h) \in \mathscr{V}$ and it is also $\mathscr{V}$ structurally stable. Since the operators $S(h)$ and $F(h)$ are topologically equivalent for sufficiently small h, see [4], we obtain that $S(t)$ and $F(h)$ are topologically equivalent for all positive values of t and h. In terms of the general theory in [2], this scheme is *topologically dynamically consistent* with the original dynamical model. Hence it preserves all topological properties of this model. In the fourth section 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 to variations in the model parameters. The last section gives some concluding remarks.

SEIR(→S) MODEL

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 (carriers which are not yet infective), I - the number of infectives and R - the number of recovered with immunity. The following mathematical model is derived in [6, Chapter 21] as a system of differential equations for the fractions of the respective classes in the total population N, that is, $u = \frac{S}{N}$, $x = \frac{E}{N}$, $y = \frac{I}{N}$, $u = \frac{R}{N}$

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

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

The system of ODEs (1) defines a dynamical system on the three dimensional closed simplex

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

Of course, one can eliminate one of the variables, e.g. u, and obtain a system of three equations. However, as it turns out, this is beneficial neither for the theoretical analysis not for the computational procedure. The point $(1,0,0,0)$ is always an equilibrium of (1). This is the Disease Free Equilibrium (DFE). The system may have another equilibrium, namely,

$$z_e = \frac{\theta\nu(\mathscr{R}_0 - 1)}{\nu + \eta - \eta\theta\mathscr{R}_0},\ \ y_e = \frac{\nu + \eta}{\theta} z_e,\ \ x_e = \frac{\nu + \theta}{\xi} y_e,\ \ u_e = 1 - x_e - y_e - z_e, \tag{2}$$

where $\mathscr{R}_0 = \frac{\xi}{(\nu+\xi)(\nu+\theta)}$ is the basic replacement ratio. The point in (2) is an equilibrium of the dynamical system (1) whenever it belongs to its domain G, that is, when $\mathscr{R}_0 > 1$. It is called an Endemic Equilibrium (EE) since it describes a permanent presence of the disease. Our concern here are the properties of the dynamical system (1). It was proved in [6, Theorem 21.2] that:

- If $\mathscr{R}_0 \leq 1$ then DFE is globally asymptotically stable on G. (3)
- If $\mathscr{R}_0 > 1$ then DFE is a hyperbolic saddle point with stable manifold $\Gamma = \{(u,x,y,z) \in G : x = y = 0\}$, EE is stable and attracting with basin of attraction $G \setminus \Gamma$. (4)

$\mathscr{V}$-STRUCTURALLY STABLE SCHEME BY THE NONSTANDARD FINITE DIFFERENCE METHOD

It is easy to see that the maps $S(t)$ for the dynamical system (1) 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 G. In order to obtain structural stability for $S(t)$ we consider the following smaller space

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

Using essentially the same method as the proof of [3, Theorem 16.3.1] we obtain for every $t > 0$ the evolution operator $S(t)$ is $\mathscr{V}$ structurally stable provided $(\nu+\xi+\theta)(\nu+\eta) > \theta\xi$. This inequality for the parameters of the model ensures that whenever DFE$\in G \setminus \Gamma$, its basin of attraction is $G \setminus \Gamma$, see [6, Theorem 21.11]. Hence it can be replaced by any other condition implying the said property, e.g. $\eta = 0$, see [6, Theorem 21.12]

The following scheme, which uses nonlocal approximation of the nonlinear term, is crafted in such a way that the operator $F(h)$ is in $\mathscr{V}$ and it is also $\mathscr{V}$ structurally stable.

$$\left\{ \begin{array}{rcl} \dfrac{u_{k+1}-u_k}{h} & = & -u_{k+1}y_k + \nu x_{k+1} + \nu y_{k+1} + (\eta+\nu)z_{k+1} \\ \dfrac{x_{k+1}-x_k}{h} & = & u_{k+1}y_k - (\xi+\nu)x_{k+1} \\ \dfrac{y_{k+1}-y_k}{h} & = & \xi x_{k+1} - (\theta+\nu)y_{k+1} \\ \dfrac{z_{k+1}-z_k}{h} & = & \theta y_{k+1} - (\eta+\nu)z_{k+1} \end{array} \right. \tag{5}$$

The method is implicit but any time step involves only the solution of a linear system

$$\begin{pmatrix} 1+hy_k & -h\nu & -h\nu & -h(\eta+\nu) \\ -hy_k & 1+h(\xi+\nu) & 0 & 0 \\ 0 & -h\xi & 1+h(\theta+\nu) & 0 \\ 0 & 0 & -h\theta & 1+h(\eta+\nu) \end{pmatrix} \begin{pmatrix} u_{k+1} \\ x_{k+1} \\ y_{k+1} \\ z_{k+1} \end{pmatrix} = \begin{pmatrix} u_k \\ x_k \\ y_k \\ z_k \end{pmatrix}. \tag{6}$$

The evolution operator of the scheme is defined through $F(h)(u_k,x_k,y_k,z_k)^T = (C(h,y_k))^{-1}(u_k,x_k,y_k,z_k)^T$, where $C(h,y_k)$ is the coefficient matrix of the linear system (6). It is easy to see that $C(h,y_k)$ is an M-matrix. Hence starting from any initial condition in G the approximations remain nonnegative for all $k = 1,2,....$ Furthermore $u_{k+1}+x_{k+1}+y_{k+1}+z_{k+1} = u_k+x_k+y_k+z_k = 1$. Therefore the scheme (5) defines a discrete dynamical system on G. One can also see that DEF and EE are preserved together with their stability. This implies that $F(h) \in \mathscr{V}$. Further, the $\mathscr{V}$ structurally stability of $F(h)$ is derived similarly to the $\mathscr{V}$ structurally stability of $S(t)$. The approximate solutions for two sets of constants are presented in Figs. 1 and 2. In Fig.1 we have $\mathscr{R}_0 = 3.9 > 1$ while in Fig. 2 $\mathscr{R}_0 = 0.93 < 1$ and one may observe that the properties of the exact solutions in (3) and (4) 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 [1], [2]. See also [5] and the references therein for a general discussion on the issue.

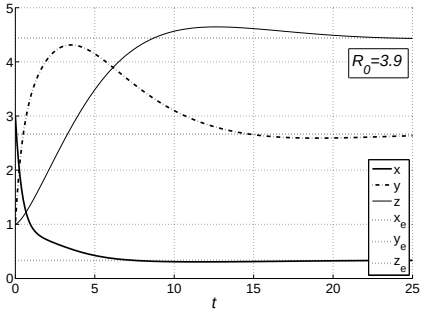

Fig. 1

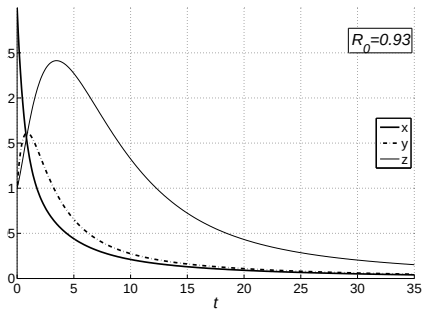

Fig. 2

SENSITIVITY ANALYSIS VIA VALIDATED COMPUTING

As mentioned in the Introduction we apply advanced methods for bounding the solution of a linear system involving interval parameters [7, 8] to (i) demonstrate quantitatively the numerical stability of the iteration scheme (6), and (ii) perform a rigorous componentwise sensitivity analysis on the model's parameters. First, we run the iteration scheme solving at each step a linear system (6) 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 (6) depends on y_k, we apply self-verified methods for solving parametric linear systems [8]. The model parameters are considered having point values $\nu = 0.2$, $\xi = 1$, $\theta = 0.7$, $\eta = 0.07$. Thus, at the first iteration step the maximal relative diameter of the intervals bounding the solution components is $5.3 * 10^{-15}$. The intervals bounding the solution get into the system at the next iteration step and thus propagate the round-off errors. Nevertheless, the maximal relative diameter at the last (351-st) iteration step is $2.6 * 10^{-11}$ showing the numerical stability of the iteration scheme. Next we estimate the sensitivity of the linear system (6) with respect to perturbations in the model parameters ν, ξ, θ, η. Let a linear system $A(p)x = b(p)$ depending on a m-tuple of parameters $p = (p_1, \ldots, p_m)$ be given, $A(p)$ 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 $[s] \in \mathbb{IR}^n$, $[s] \supseteq \Sigma(A(p), b(p), [p])$, $f := \mathrm{rad}([s])/\varepsilon \geq \mathrm{rad}(\Sigma(A(p), b(p), [p]))/\varepsilon$ 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 run the iteration scheme solving at each step the system (6) with $\varepsilon = 10^{-12}$ for the perturbed model parameters. Table 1 displays f for the solution components at the last iteration step. In contrast to a single condition number given by the classical sensitivity analysis, we perform a componentwise sensitivity analysis of the solution. As shown in Table 1, some individual solution components are much more responsive to small perturbations in the input parameters than others. Due to an automatic error control mechanism the accuracy of every computed result is guaranteed. It is shown in [9] that traditional condition numbers do not necessarily reflect the true sensitivity of the solution components.

TABLE 1. Componentwise sensitivity ($10f$)

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

CONCLUSION

This paper brings together two methods of producing numerical solutions with a statement of their quality - the non-standard finite difference method and the method of validated computing. Their combined application is demonstrated of 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.

REFERENCES

1. R. Anguelov, Dynamically Consistent Schemes for Epidemiological Models, *Proceedings of the Annual Meeting of the Bulgarian Section of SIAM, 22-23 December 2008, Sofia*, Demetra, Sofia, 2009, 11–14
2. R. Anguelov, J.M.-S. Lubuma and M. Shillor, Dynamically consistent nonstandard finite difference schemes for continuous dynamical systems, *AIMS Proceedings*, to appear.
3. M.W. Hirsch, S. Smale, *Differential equations, dynamical systems and linear algebra*, Academic Press, New York, 1974.
4. M-C Li, Structural stability for the Euler method, *SIAM Journal of Mathematical Analysis* **30**, 747–755 (1999).
5. R.E. Mickens (Ed), *Advances in the applications of nonstandard finite difference schemes*, World Scientific, Singapore, 2005.
6. H.R. Thieme, *Mathematics of population biology*, Princeton University Press, Princeton and Oxford, 2003.
7. Popova, E.D., Parametric Interval Linear Solver, *Numerical Algorithms* **37**, 345–356 (2004).
8. Popova, E.D., Krämer, W., Inner and Outer Bounds for Parametric Linear Systems, *Journal of Computational and Applied Mathematics* **199**, 310–316 (2007).
9. S. Rump, Rigorous sensitivity analysis for systems of linear and nonlinear equations, *Mathematics of Computation* **54**, 721–736 (1990).