SHORT NOTE

# On the symmetrization and composition of nonstandard finite difference schemes as an alternative to Richardson's extrapolation

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**ABSTRACT**
From the classical explicit Euler scheme of first order, nonstandard finite difference (NSFD) schemes were envisioned to mimic the essential properties of the governing differential equation model for every time step-size. In the context of compartmental epidemiological models, these properties are generally concerned with positivity of subpopulations, conservation laws (dynamics of the total population), and stability. However, for autonomous systems, the symmetry (self-adjoint) condition is not preserved. Compartmental epidemiological models are Poisson systems, so methods from geometric numerical integration should be applicable. It is found out that symmetrization of NSFD schemes does not respect positivity for every step-size, though other characteristics are maintained and second order is reached. Composition through the Lie formalism can then be applied to obtain higher-order schemes. This is a more efficient and consistent alternative to Richardson's extrapolation, which has often been used to go beyond order one.

**KEYWORDS**
Mickens' nonstandard finite difference scheme; structure preservation and consistency; symmetrization; higher-order integrators via composition; autonomous compartmental epidemiological model; Richardson's extrapolation; efficiency

## 1. Introduction

It is known that most of the models formulated by differential equations do not possess closed-form solutions, which makes the use of numerical methods necessary. Differential equation models may have some underlying structure, so it seems natural to design numerical integrators that preserve it. The motivation is not only the improvement of the qualitative behavior, but also the accuracy provided compared to general-purpose methods.

With this aim, R.E. Mickens suggested a new field of research involving nonstandard finite difference (NSFD) schemes [1–4]. This dates back to twenty–thirty years ago, and it is still a very active area of research [5–8]. Essentially, two principles are followed: from the classical explicit Euler (or forward Euler) scheme of first order, nonlocal discretizations are set and the classical denominator for the discretization of the first-order derivative is modified. In the setting of compartmental epidemiological models [9], nonlocal discretizations help ensuring the positivity of the subpopulations. These nonlocal discretizations usually make the scheme half way between an explicit

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and an implicit formulation, which confers it stability. Explicit standard schemes (Euler, Heun, Runge-Kutta, etc.) may fail at reproducing the correct dynamics for some step-sizes, which may be especially problematic for stiff problems. On the other hand, the new denominator functions for the discretization of the first-order derivative are selected according to conservation laws, normally related to the dynamics of the total population, and on the basis of exact schemes for basic models. See [10–12]. To summarize, NSFD discretizations of compartmental epidemiological models are concerned with positivity, stability and conservation laws. Often, after algebraic manipulations, NSFD schemes can be written explicitly, so that they can be easily run compared with traditional implicit standard schemes [8].

NSFD schemes are of first order. To achieve higher order, the application of Richardson's extrapolation (RE) [13] was proposed [14, 15]. The correction to remove the leading-order error term may not respect positivity for every step-size, although other characteristics are maintained. Because of convergence, positivity holds for sufficiently small step-size on any bounded time domain, albeit the positivity threshold is generally unknown.

When the compartmental epidemiological model is autonomous, the symmetry (or self-adjointness) of the solution is not conserved by NSFD schemes. This feature, along with others, are taken into account in the context of Hamiltonian dynamics by geometric numerical integration (GNI) [16, 17]. The symplectic character of the solution, rather than the invariability of mechanical energy (conservation law), is always preserved, giving rise to symplectic integrators. Whenever possible, reversibility of the flow is mimicked as well. GNI constructs high-order methods by composition and splitting. When the Hamiltonian system is noncanonical, one refers to Poisson systems and works with Poisson integrators, which respect the associated Casimir functions and the Poisson character of the flow. Compartmental epidemiological models are Poisson, as shown thirty years ago for the SIR model [18] and recently generalized [19].

In this brief note, the symmetry of NSFD schemes is studied. As is well-known, symmetric integrators must be of even order, so the NSFD schemes of order one cannot be symmetric. In GNI, the usual procedure to transform a nonsymmetric method into a symmetric one consists in composing with the adjoint version. But it is not clear which properties of the NSFD scheme are still preserved. Also studied here is the composition procedure from GNI to generate higher-order NSFD integrators. In conclusion, it is of interest to investigate the relation between NSFD integration and GNI, as both rely on preserving the structure of the governing model. A comparison with RE, in terms of consistency and cost, is performed in detail. A numerical example on an autonomous SIRS model is conducted, where different selections of input parameters yield non-stiff and stiff equations.

## 2. Symmetrization and composition of NSFD schemes

In the context of autonomous systems, $\dot{x} = f(x)$, $x \in \mathbb{R}^d$, the flow $\varphi_t(x)$ satisfies a symmetry condition: $\varphi_t = \varphi_{-t}^{-1}$. NSFD schemes are not symmetric. That is, if $\mathcal{X}_h(x)$ is the map of the NSFD scheme with step-size $h$ (i.e. the scheme reads recursively as $x_{N+1} = \mathcal{X}_h(x_N)$), then $\mathcal{X}_h \neq \mathcal{X}_{-h}^{-1}$. Indeed, being of order one prevents from satisfying this property [17] (see the first appendix). Also, higher-order schemes cannot be constructed by composition. For instance, a usual strategy from GNI to build higher-order

integrators [17] is to compose

$$\psi_h = \mathcal{X}_{\gamma_s h} \circ \mathcal{X}_{\gamma_{s-1} h} \circ \cdots \circ \mathcal{X}_{\gamma_1 h},$$

where $\gamma_1, \ldots, \gamma_s$ are selected appropriately. It is known that $\mathcal{X}_h(x) = \mathrm{e}^{X(h)}[\mathrm{Id}](x)$, where $X(h) = \sum_{n=1}^{\infty} h^n X_n$ is an operator, with $X_1 = L_f = \sum_{i=1}^{d} f_i \frac{\partial}{\partial x_i}$ being the Lie derivative of $f$, and $X_2 \neq 0$. By the BCH formula, which expresses $\mathrm{e}^X \mathrm{e}^Y = \mathrm{e}^{Z(X,Y)}$ for any two operators $X$ and $Y$ (see the second appendix), it is obtained $\gamma_1 + \ldots + \gamma_s = 1$ and $\gamma_1^2 + \ldots + \gamma_s^2 = 0$. Thus, it is not possible to apply composition for a first-order NSFD scheme. It would be necessary that $\mathcal{X}_h$ be of even order $r$, as in such a case $X_1 = L_f$, $X_n = 0$ for $2 \leq n \leq r$, and the conditions

$$\gamma_1 + \ldots + \gamma_s = 1, \quad \gamma_1^{r+1} + \ldots + \gamma_s^{r+1} = 0 \tag{1}$$

can hold to achieve a new method $\psi_h$ of order at least $r + 1$.

In order for the NSFD scheme to be symmetric, one considers the adjoint $\mathcal{X}_h^* = \mathcal{X}_{-h}^{-1}$ and defines $\mathcal{S}_h = \mathcal{X}_{h/2}^* \circ \mathcal{X}_{h/2}$ (analogously, $\mathcal{X}_{h/2} \circ \mathcal{X}_{h/2}^*$). The adjoint is easily computable, by replacing $x_{N+1} \leftrightarrow x_N$ and $h \leftrightarrow -h$ in the scheme $x_{N+1} = \mathcal{X}_h(x_N)$. The new scheme $\mathcal{S}_h$ is symmetric ($\mathcal{S}_h = \mathcal{S}_{-h}^{-1}$) and of order two. Each iteration of step-size $h$ is computed by first applying the NSFD scheme with step-size $h/2$ and afterward its adjoint scheme with step-size $h/2$. In the setting of compartmental epidemiological models, the symmetrization does not respect the positivity of $\mathcal{X}_h$ independently of the step-size, though conservation laws and stability are maintained. It is not clear whether either symmetry or positivity should be preferred. At least, due to convergence, it is evident that positivity holds for sufficiently small step-size $h$ on any bounded time domain, albeit the positivity threshold is generally unknown.

Since $\mathcal{S}_h$ is of second order, the symmetric composition

$$\psi_h = \mathcal{S}_{\alpha h} \circ \mathcal{S}_{\beta h} \circ \mathcal{S}_{\alpha h} \tag{2}$$

can be employed, with $\alpha = 1/(2 - 2^{1/3})$ and $\beta = 1 - 2\alpha$ (check (1) with $s = 3$, $\gamma_1 = \gamma_3 = \alpha$, $\gamma_2 = \beta$). This new method $\psi_h$ is of fourth order and symmetric. Further, conservation laws and stability hold. Each iteration of step-size $h$ is computed by first applying $\mathcal{S}$ with step-size $\alpha h$, then $\mathcal{S}$ with step-size $\beta h$, and finally $\mathcal{S}$ with step-size $\alpha h$.

In conclusion, the strategies from GNI may be used for NSFD integration, but positivity may be lost for moderate step-sizes in favor of symmetry, conservation laws and higher order through composition.

Some open questions are the following:

1. Given an autonomous compartmental epidemiological model, do there exist efficient second-order NSFD schemes that satisfy symmetry, positivity, stability and respect conservation laws? In such a case, composition methods would be applicable to increase the order.
2. Given a compartmental epidemiological model, would it be better to treat it as a Poisson system and use methods from GNI, instead of the NSFD methodology? In which situations do the same schemes arise?

## 3. Comparison with RE

Compared to RE, $\mathcal{S}_h$ is symmetric. Both methods respect the conservation law, but not the positivity for every step-size. Thus, $\mathcal{S}_h$ is more consistent.

RE with step-size $h$ at a time $T$ is defined here as twice the first-order approximation at $T$ with step-size $h/2$, minus the first-order approximation at $T$ with step-size $h$. Let us see that the computational cost of $\mathcal{S}_h$ is lower than that of RE. Let $c$ be the cost, defined as the number of arithmetic operations, of an evaluation $(h', x) \mapsto \mathcal{X}_{h'}(x)$. The cost is approximately equal for any $h'$ and $x$, therefore $c$ is assumed constant. A single evaluation $(h', x) \mapsto \mathcal{S}_{h'}(x)$ costs $2c$, by composition. At time $T$ and with step-size $h$, for which $T/h$ steps are required (assuming divisibility), the total cost of $\mathcal{S}_h$ is $c_{\mathcal{S}_h} = 2cT/h$. By contrast, the total cost of RE is $c_{\mathrm{RE},h} = 2cT/h + cT/h = 3cT/h$ (first-order approximation with step-size $h/2$, and first-order approximation with step-size $h$). In conclusion,

$$c_{\mathrm{RE},h} = \frac{3}{2} c_{\mathcal{S}_h}.$$

Similarly, one evaluation $(h', x) \mapsto \psi_{h'}(x)$ costs $6c$, by composition (recall (2)). At time $T$ and with step-size $h$, the total cost of $\psi_h$ is $c_{\psi_h} = 6cT/h$. The application of three RE (to achieve order four) costs $c_{\mathrm{RE}\circ\mathrm{RE}\circ\mathrm{RE},h} = 27cT/h$. In consequence,

$$c_{\mathrm{RE}\circ\mathrm{RE}\circ\mathrm{RE},h} = \frac{9}{2} c_{\psi_h}.$$

As the order increases, the ratio of costs tends to infinity. Notice the these estimates do not depend on the implementation or the computer.

## 4. A SIRS model

### *4.1. The model*

Consider the following SIRS model with vital dynamics:

$$\dot{S}(t) = \mu - \mu S(t) - \beta S(t) I(t) + \gamma R(t),$$

$$\dot{I}(t) = \beta S(t) I(t) - \nu I(t) - \mu I(t),$$

$$\dot{R}(t) = \nu I(t) - \gamma R(t) - \mu R(t),$$

where $S(t)$, $I(t)$ and $R(t)$ are the proportions of susceptible, infected and recovered individuals at time $t \geq 0$. The coefficients are positive and time invariant. The total population, $P(t) = S(t) + I(t) + R(t)$, satisfies $\dot{P} = \mu(1 - P)$. This is a conservation law. When $P(0) = 1$, the equality $P(t) = 1$ holds for all $t$. If $P(0) < 1$, then $P(\infty) = 1$. (This latter case is studied when there are two disjoint groups $P(t)$ and $P'(t)$ in the population, the investigation is focused on $P$, and all the newborns from parents in $P'$ enter into $P$ automatically.)

### *4.2. The numerical schemes*

In [5], the NSFD methodology was applied (when $\beta$ is dependent on $t$, but here it is assumed invariant to have an autonomous system). The discretization is the following:

$$\frac{S_{N+1}-S_N}{\phi(h)} = \mu - \mu S_{N+1} - \beta S_{N+1} I_N + \gamma R_{N+1},$$

$$\frac{I_{N+1}-I_N}{\phi(h)} = \beta S_{N+1} I_N - \nu I_{N+1} - \mu I_{N+1},$$

$$\frac{R_{N+1}-R_N}{\phi(h)} = \nu I_{N+1} - \gamma R_{N+1} - \mu R_{N+1}.$$

The step-size is $h$. The nonlocal discretizations ensure positivity. The denominator function is

$$\phi(h) = \frac{\mathrm{e}^{\mu h}-1}{\mu},$$

which gives an exact scheme for $P(t)$, irrespective of the step-size $h$ and the initial condition $P(0)$:

$$\frac{P_{N+1}-P_N}{\phi(h)} = \mu(1-P_{N+1}). \tag{3}$$

As shown in [5], the scheme can be written explicitly, so that $(S_{N+1}, I_{N+1}, R_{N+1}) = \mathcal{X}_h(S_N, I_N, R_N)$ in closed form. Consider $\mathcal{S}_h = \mathcal{X}^*_{h/2} \circ \mathcal{X}_{h/2}$ and $\psi_h$ through (2). Even though $\mathcal{S}_h$ can be expressed in closed form, with huge formulas, in a symbolic software, both $\mathcal{S}_h$ and $\psi_h$ can (and should) be run numerically through the compositions.

### *4.3. Comparison with RE*

Some numerical experiments are performed, for fixed data $\mu = 1$, $\nu = 0.01$, $\beta = 3$, $\gamma = 10$, $S(0) = 0.8$, $I(0) = 0.1$ and $R(0) = 0.1$. Four methods are used: $\mathcal{X}_h$, $\mathcal{S}_h$, $\psi_h$ and $\mathrm{RE}_h$. For $h = 1$, $\mathcal{S}_h$ and RE give negative values for $R(1)$ ($S(1)$ is negative under $\mathcal{S}_h$ too), which demonstrates that the symmetrization and the RE do not conserve positivity for some $h$. However, the conservation law (3) is obeyed. In Figure 1, the absolute errors between $S(t)$ and $S_N$ are reported, at $t = 3$ (first panel) and $t = 8$ (second panel). Step-sizes $h = 2^{-j}$, $j \geq 0$, are taken. Double logarithmic scale is set, in accordance with algebraic convergence. On the other hand, in terms of required cost, recall that cost $= kc \cdot 3/h$ ($t = T = 3$), where $c \approx$ constant is the number of arithmetic operations of any evaluation $(h', x) \mapsto \mathcal{X}_{h'}(x)$, and $k = 1$, $k = 2$, $k = 3$ and $k = 6$ for $\mathcal{X}_h$, $\mathcal{S}_h$, RE with $h$ and $\psi_h$, respectively. Figure 2 plots cost$/(3c) = k/h$ against the absolute errors between $S(t)$ and $S_N$, for $t = 3$ (first panel) and $t = 8$ (second panel). Notice that cost$/(3c)$ is equal to $1/h$, $2/h$, $3/h$ and $6/h$ for $\mathcal{X}_h$, $\mathcal{S}_h$, RE with $h$ and $\psi_h$, respectively. The plot compares computational effort with accuracy, rather than step-size with accuracy; it is an efficiency plot. It is observed that the symmetrization $\mathcal{S}_h$

gives lower error than the RE for the same cost. Thus, symmetrization and composition of NSFD schemes seems to be a good alternative to RE.

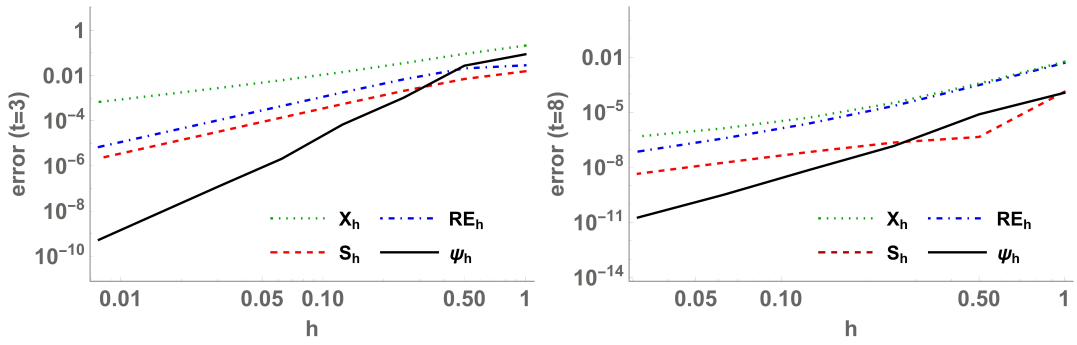


**Figure 1.** Comparison of the methods in terms of the step-size value $h$: $\mathcal{X}_h$ (first-order NSFD scheme), $\mathcal{S}_h$ (second-order symmetrization $\mathcal{X}^*_{h/2} \circ \mathcal{X}_{h/2}$), $\psi_h$ (fourth-order composition of $\mathcal{S}_h$ through the Lie formalism), and second-order RE on $\mathcal{X}_h$. Inputs: $\mu = 1$, $\nu = 0.01$, $\beta = 3$, $\gamma = 10$, $S(0) = 0.8$, $I(0) = 0.1$ and $R(0) = 0.1$. First panel: $t = 3$. Second panel: $t = 8$. Absolute errors between $S(t)$ and $S_N$ are reported.

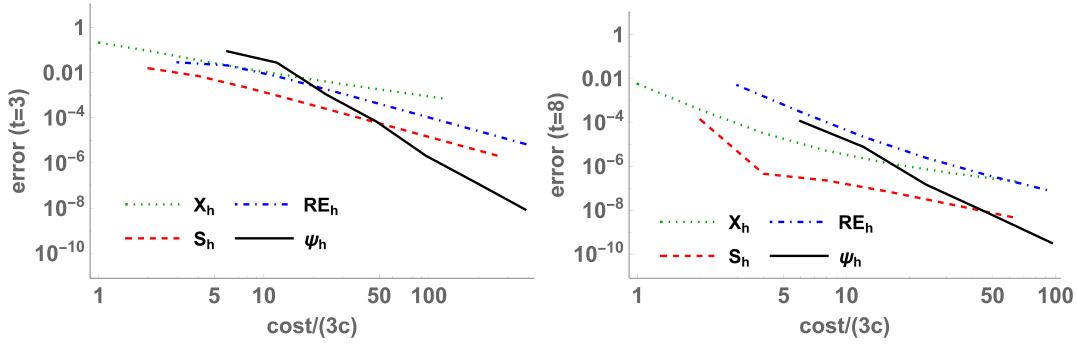


**Figure 2.** Same as Figure 1, but with respect to the cost. Efficiency plot.

### *4.4. Comparison with explicit standard schemes: A non-stiff problem*

Implicit standard schemes were designed to overcome the disadvantages of explicit standard methods in terms of stability. An important feature of NSFD schemes is that these are written explicitly, in contrast to implicit standard schemes, but still maintain stability due to the nonlocal discretizations. In this regard, Figure 3 aims at showing the instability of explicit Euler and Runge-Kutta methods, compared to the nonstandard methods proposed in the present paper. We fix $h = 0.3$ and $h = 0.5$, for the same parameter values as before: $\mu = 1$, $\nu = 0.01$, $\beta = 3$, $\gamma = 10$, $S(0) = 0.8$, $I(0) = 0.1$ and $R(0) = 0.1$.

### *4.5. Comparison with explicit standard schemes: A stiff problem*

As it occurs with implicit standard schemes, the main advantage of NSFD schemes over explicit standard schemes arises when the model is stiff. We vary the input parameters from the previous two subsections, so that very slow and very fast transition rates

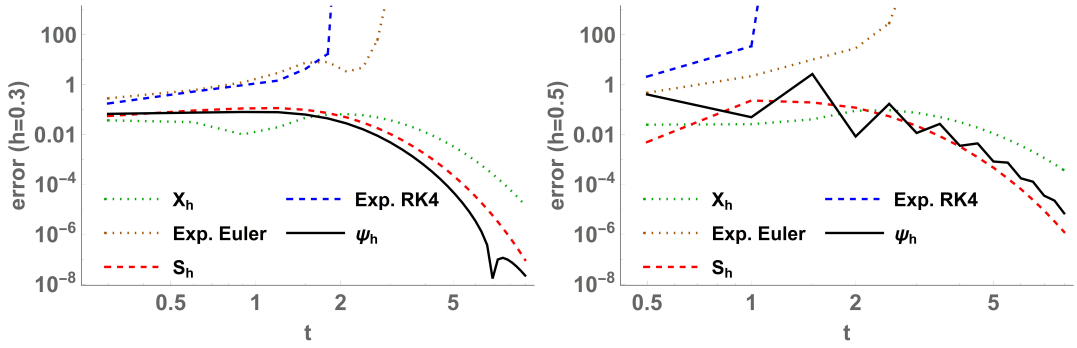


**Figure 3.** Comparison of the methods in terms of stability: $\mathcal{X}_h$ (first-order NSFD scheme), $\mathcal{S}_h$ (second-order symmetrization $\mathcal{X}^*_{h/2} \circ \mathcal{X}_{h/2}$), $\psi_h$ (fourth-order composition of $\mathcal{S}_h$ through the Lie formalism), second-order RE on $\mathcal{X}_h$, explicit Euler, and explicit Runge-Kutta RK4. Inputs: $\mu = 1$, $\nu = 0.01$, $\beta = 3$, $\gamma = 10$, $S(0) = 0.8$, $I(0) = 0.1$ and $R(0) = 0.1$. Non-stiff case. First panel: $h = 0.3$. Second panel: $h = 0.5$. Absolute errors between $S(t)$ and $S_N$ are reported.

between compartments coexist. Let $\mu = 0.001$, $\nu = 0.001$, $\beta = 0.001$, $\gamma = 10000$, $S(0) = 0.8$, $I(0) = 0.1$ and $R(0) = 0.1$. In Figure 4, we illustrate how explicit standard schemes exhibit growing error for $h = 0.0005$, in contrast to NSFD methods. Let us comment that the degree of stiffness of the problem may be increased as strongly as wanted, so that the threshold $h$ for which explicit standard schemes work is made lower and lower.

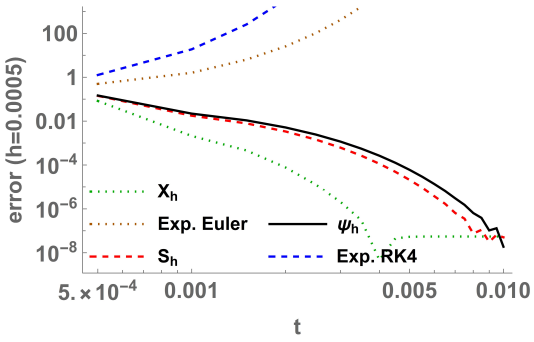


**Figure 4.** Comparison of the methods in terms of stability: $\mathcal{X}_h$ (first-order NSFD scheme), $\mathcal{S}_h$ (second-order symmetrization $\mathcal{X}^*_{h/2} \circ \mathcal{X}_{h/2}$), $\psi_h$ (fourth-order composition of $\mathcal{S}_h$ through the Lie formalism), second-order RE on $\mathcal{X}_h$, explicit Euler, and explicit Runge-Kutta RK4. Inputs: $\mu = 0.001$, $\nu = 0.001$, $\beta = 0.001$, $\gamma = 10000$, $S(0) = 0.8$, $I(0) = 0.1$ and $R(0) = 0.1$. Stiff case, $h = 0.0005$. Absolute errors between $S(t)$ and $S_N$ are reported.

## 5. Conclusion

NSFD schemes are dynamically consistent, but are of first order as originally formulated. In the literature, higher-order constructions were proposed from RE. The essential properties of the governing system were thus maintained, except maybe the positivity condition regardless of the step-size value. In this short note, an alternative approach is suggested. For autonomous systems, the NSFD scheme can be symmetrized by composing with the adjoint scheme, so that the symmetry condition of the exact

solution is mimicked. This is the usual procedure in GNI. It gives rise to an explicit second-order method, which preserves all properties (symmetry, conservation laws, stability) unconditionally except positivity for every step-size. Composition through the Lie formalism allows increasing the order of the method. Here it is stopped at fourth order. The symmetric method is more efficient and consistent than RE. For a fixed step-size value, the ratio of costs is 3/2, independently of the implementation and the computer. If fourth-order methods are compared, namely composition of three symmetrizations and composition of three RE, then the ratio of costs is 9/2. The ideas are illustrated on an autonomous SIRS model, albeit analogous applications may be conducted for other epidemiological models such as SIS, SEIR, etc.

In the future, the link between NSFD integration and GNI shall be studied further, as the connection is still under-investigated. This would also help to solve the two open questions posed in this work. On the other hand, different compartmental problems with many subgroups and strong stiffness shall be tackled in the future, as the potential of NSFD schemes (with symmetrization and composition) will likely be the biggest. Implicit standard schemes, whose usefulness is very significant, were designed to overcome the disadvantages of explicit standard methods in terms of stability. NSFD schemes achieve this target due to the nonlocal discretizations, while being explicit, positivity preserving / symmetric and conservation-law preserving. Thus, NSFD methods have advantages compared to standard methods and deserve further research.

## Appendix A

NSFD schemes of order one, and in general of odd order, cannot preserve symmetry: $\mathcal{X}_h \neq \mathcal{X}_h^*$, where $\mathcal{X}_h^* = \mathcal{X}_{-h}^{-1}$ is the adjoint. Let us justify this statement. It is known that $\mathcal{X}_h(x) = \mathrm{e}^{X(h)}[\mathrm{Id}](x)$, where $X(h) = \sum_{n=1}^{\infty} h^n X_n$ and $X_1 = L_f$. The scheme is of order $r$ if and only if $X_n = 0$ for $2 \leq n \leq r$. On the other hand, $\mathcal{X}_h^*(x) = \mathrm{e}^{-X(-h)}[\mathrm{Id}](x)$, where $-X(-h) = \sum_{n=1}^{\infty}(-1)^{n+1} h^n X_n$. Thus, $\mathcal{X}_h = \mathcal{X}_h^*$ if and only if $X_n = 0$ whenever $n$ is even, that is, $X(h) = hX_1 + h^3 X_3 + h^5 X_5 + \ldots$; this is equivalent to $\mathcal{X}_h$ being of even order $r$.

## Appendix B

The BCH (Baker-Campbell-Hausdorff) formula expresses $\mathrm{e}^X \mathrm{e}^Y = \mathrm{e}^{Z(X,Y)}$ for any two operators $X$ and $Y$. From $\mathrm{e}^X \mathrm{e}^Y = \sum_{m,n=0}^{\infty} \frac{1}{m!n!} X^m Y^n$ and the power series expansion of the logarithm function, $Z = \log(\mathrm{e}^X \mathrm{e}^Y) = \sum_{m=1}^{\infty} Z_m(X,Y)$ is obtained. The computation of the explicit series is not simple. The terms are usually expressed in terms of the commutator $[X,Y] = XY - YX$:

$$Z_1(X,Y) = X + Y, \quad Z_2(X,Y) = \frac{1}{2}[X,Y],$$

$$Z_3(X,Y) = \frac{1}{12}\left([X,[X,Y]] - [Y,[X,Y]]\right), \quad Z_4(X,Y) = -\frac{1}{24}[Y,[X,[X,Y]]].$$

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## Conflict of Interest Statement

The authors declare that there is no conflict of interests regarding the publication of this article.

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