Operator splitting methods
for the Lotka–Volterra equations

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Abstract. Geometric integrators are numerical methods for differential equations that preserve geometric properties. In this article we investigate the questions of constructing such methods for the well-known Lotka–Volterra predator–prey system by using the operator splitting method. We use different numerical methods combined with the operator splitting method and analyse if they preserve the geometric properties of the original system.

Keywords: numerical methods, operator splitting, Hamilton systems, Lotka–Volterra equations.

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1   Preliminary

By modelling different phenomena in the nature, it is one of the most important factors to preserve their qualitative properties. These properties are derived from certain fundamental (biological, physical, etc) laws. Such attributes include the preservation of the energy, phase space volume, symmetry and symplectic structure. In several cases the standard numerical methods ignore all these laws, models. Therefore it is important to use numerical methods that preserve such properties.

1.1   Mathematical background

First, we investigate the attributes of the continuous problem, the Hamiltonian and Poisson systems and their geometric properties. These notations are the first integral, the simplecticity, the volume preservation and the Poisson map.

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Definition 1.1. Let $D \subset \mathbb{R}^d$ be a given domain and $f : D \to \mathbb{R}^d$ some given continuous mapping and $y_0 \in \mathbb{R}^d$ a given vector. The problem

$$\frac{dy(t)}{dt} = f(y(t)) \tag{1.1}$$

$$y(0) = y_0 \tag{1.2}$$

is called initial value problem or Cauchy problem for an autonomous system.

We assume that the function f is Lipschitz continuous, then the Cauchy problem (1.1)–(1.2) has a unique solution.

Definition 1.2. A differentiable map $\mathcal{G} : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ is called symplectic if its Jacobian matrix is everywhere symplectic i.e.,

$$(\mathcal{G}'(y))^T J \mathcal{G}'(y) = J, \qquad \forall y \in \text{dom}(\mathcal{G}), \tag{1.3}$$

where

$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \tag{1.4}$$

and $I \in \mathbb{R}^{d \times d}$ denotes the identity matrix .

Definition 1.3. A map $\mathcal{G} : D \to \mathbb{R}^d$ is called an area-preserving transformation if for any bounded $\Sigma \in \text{dom}(\mathcal{G})$ domain, Σ and $\mathcal{G}(\Sigma)$ have the same area.

Proposition 1.4 ([4])**.** *If $\mathcal{G} : D \to \mathbb{R}^d$ is a symplectic map, then it is an area-preserving transformation.*

Definition 1.5. The exact flow $\Phi_t : D \to \mathbb{R}^d$ of the problem (1.1)–(1.2) is defined as

$$\Phi_t(y_0) = y(t). \tag{1.5}$$

Definition 1.6. A first integral of the problem (1.1) is a non-constant continuously differentiable function $\mathcal{I} : \mathbb{R}^d \to \mathbb{R}$, such that

$$\mathcal{I}(y)|_{y=y(t)} = \text{Constant} \tag{1.6}$$

for any $y(t)$ solving the equation (1.1).

This means that the function $\mathcal{I}$ is constant along the solutions to (1.1). Hence, some non-constant differentiable function $\mathcal{I}(y)$ is a first integral of the problem (1.1) if and only if

$$\frac{d}{dt}\mathcal{I}(y(t)) = 0 \qquad \forall y(t) \text{ solving (1.1)}. \tag{1.7}$$

The first integral plays important roles in theory of dynamical systems. It is particularly studied in the theory of Hamiltonian systems.

Definition 1.7. A Hamiltonian system for the unknown functions $p, q : \mathbb{R}_0^+ \to \mathbb{R}^d$ is a system of the form

$$\begin{cases} \dfrac{dp(t)}{dt} = -\dfrac{\partial H(p(t), q(t))}{\partial q} \\[2mm] \dfrac{dq(t)}{dt} = \dfrac{\partial H(p(t), q(t))}{\partial p} \end{cases} \tag{1.8}$$

where $H : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is a smooth function. Such a dynamical system is called a Hamiltonian system and H is called the Hamiltonian function of the system.

Hamiltonian systems play an important role in the theory of dynamical systems and it is used in numerous fields. E.g., in mechanics a Hamiltonian system describes the motion involving constraints and forces which have a potential. Hamiltonian systems have a broad literature, see e.g. [4, 9]. In the following, we investigate the main attributes of such systems. The Hamilton function usually represents the total energy of the system.

Proposition 1.8. *The function $H(p,q)$ is the first integral of the system* (1.8).

Proof. Using the chain rule, we have

$$\frac{d}{dt}H(p(t),q(t)) = \sum_{i=1}^{d} \frac{\partial H}{\partial p_i} \cdot \frac{dp_i}{dt} + \frac{\partial H}{\partial q_i} \cdot \frac{dq_i}{dt}$$
$$= \sum_{i=1}^{d} \frac{\partial H}{\partial pi} \cdot \left(-\frac{\partial H}{\partial q_i}\right)^T + \frac{\partial H}{\partial q_i} \cdot \left(\frac{\partial H}{\partial p_i}\right)^T = 0,$$

which proves the statement. $\square$

One of the most important properties of Hamiltonian systems is the symplecticity of their flow.

Theorem 1.9 ([4]). *Let $H(p,q)$ be a twice continuously differentiable function. Then for each fixed t the flow of the Hamiltonian system* (1.8) *is a symplectic transformation wherever it is defined.*

In the following we define the Poisson bracket, that is used in the theory of Lie algebra and with this notation we investigate the generalized Hamiltonian systems.

Definition 1.10. The Poisson bracket $\{\cdot, \cdot\}$ of two functions $F(p,q), G(p,q) : C^1(\mathbb{R}^d \times \mathbb{R}^d) \to \mathbb{R}$ is defined as

$$\{F, G\} = \sum_{i=1}^{d} \left(\frac{\partial F}{\partial q_i} \frac{\partial G}{\partial p_i} - \frac{\partial F}{\partial p_i} \frac{\partial G}{\partial q_i}\right), \tag{1.9}$$

or in a more compact form $\{F, G\}(y) = \nabla F(y)^T J^{-1} \nabla G(y)$, where $y = (p,q)$ and J is the matrix in (1.4).

We note that p and q usually denote the generalized coordinates and in certain sense the Poisson bracket yields the analogue of the commutator.
The Poisson bracket satisfies the Lie bracket axioms, i.e. it has the bi-linearity, Jacobi identity, Leinbniz's rule and anti-commutativity properties. It is easy to see that the first integral of a Hamiltonian system can be characterized with the help of the Poisson bracket as follows.

Proposition 1.11 ([4]). *A function $\mathcal{I}(p,q)$ is a first integral of the problem* (1.8) *if and only if*

$$\{\mathcal{I}, H\} = 0. \tag{1.10}$$

Let us define the generalization of the Hamiltonian system, which also has many applications.

Definition 1.12. Let $B(y)$ be a skew-symmetric matrix with the property

$$\sum_{l=1}^{n} \left(\frac{\partial b_{ij}(y)}{\partial y_l} b_{lk}(y) + \frac{\partial b_{jk}(y)}{\partial y_l} b_{li}(y) + \frac{\partial b_{ki}(y)}{\partial y_l} b_{lj}(y) \right) = 0, \tag{1.11}$$

for all i, j, k.

Then the formula

$$\{F, G\}_B (y) = \sum_{i,j=1}^{n} \left(\frac{\partial F(y)}{\partial y_i} b_{ij}(y) \frac{\partial G(y)}{\partial y_j} \right) \tag{1.12}$$

is said to represent a general Poisson bracket. The corresponding differential system

$$\dot{y} = B(y) \nabla H(y) \tag{1.13}$$

is called a Poisson system.

Clearly, when $B(y) = J^{-1}$, than the Poisson system turns into the Hamiltonian system.

Definition 1.13. A continuously differentiable function C is called a Casimir function of the Poisson system (1.13) if

$$C(y(t)) = \text{Constant} \tag{1.14}$$

for any $y(t)$ solving the problem (1.13).

A Casimir function is a first integral of a Poisson system with structure matrix $B(y)$, whatever the Hamiltonian $H(y)$ is. Clearly, for the Casimir function $C(y)$ of the system (1.13), we have

$$\{C, H\}_B (y(t)) = 0 \tag{1.15}$$

for all $y(t)$ solving (1.13). Obviously, the function $H(y)$ is a Casimir function of system (1.13).

The flow of the Poisson system (1.13) satisfies a property closely related to symplecticity.

Definition 1.14. A transformation $\mathcal{G} : U \to \mathbb{R}^d$, $U \subset \mathbb{R}^d$ is called a Poisson map if its Jacobian matrix satisfies

$$(\mathcal{G}'(y))^T B(y) \mathcal{G}'(y) = B(\mathcal{G}(y)). \tag{1.16}$$

Theorem 1.15 ([4]). *If $B(y)$ is the structure matrix of a Poisson bracket, then the flow Φ_t of the Poisson system (1.13) is a Poisson map.*

1.2 An important application: the Lotka–Volterra system

We analyze the above properties on the well-known population dynamical model, namely on the Lotka–Volterra system. This system is a pair of first-order, nonlinear differential equations used to describe the dynamics of biological systems, in which two species interact. The model is a basis model in population dynamics and it has various extensions [2,6,8]. If $N(t)$ denotes the prey population and $P(t)$ is the predator population at time t, respectively, then the system has the form

$$\begin{cases} \dfrac{dN}{dt} = aN - bNP, \\ \dfrac{dP}{dt} = cNP - dP, \end{cases} \tag{1.17}$$

where a, b, c and d are positive constants.

In this model, it is assumed that the prey population has an unlimited food, and it grows exponentially without predators. This exponential growth is represented in the equation by the term aN. We assume that the rate of the predation depends on the rate at which the predators and prey meet, this is represented by bNP. In the equation for the predators, cNP represents the growth rate of the population. The term dP is the loss of the predators, which leads to the exponential decay in the absence of prey. Hence the equation of the predators expresses the change of the population as growth rate minus natural death.

If we introduce the function $V : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$, defined as

$$V(N, P) = cN - d \ln N + bP - a \ln P, \tag{1.18}$$

the Lotka–Volterra system can be rewritten in the form

$$\begin{cases} \dfrac{dN}{dt} = -NP \dfrac{\partial V}{\partial P} \\ \dfrac{dP}{dt} = NP \dfrac{\partial V}{\partial N}, \end{cases} \tag{1.19}$$

i.e., with the choice

$$B(N, P) = \begin{pmatrix} 0 & -NP \\ NP & 0 \end{pmatrix} \tag{1.20}$$

it is a Poisson system. However, using the logarithmic transformations

$$\tilde{N} = \ln N, \qquad \tilde{P} = \ln P, \tag{1.21}$$

which transforms $V(N, P)$ to $H(\tilde{N}, \tilde{P}) = ce^{\tilde{N}} + be^{\tilde{P}} - a\tilde{P} - d\tilde{N}$, the Lotka–Volterra system becomes a Hamiltonian system of the form

$$\begin{cases} \dfrac{d\tilde{N}}{dt} = \dfrac{1}{N} \dfrac{dN}{dt} = -\dfrac{\partial H}{\partial \tilde{P}}, \\ \dfrac{d\tilde{P}}{dt} = \dfrac{1}{P} \dfrac{dP}{dt} = \dfrac{\partial H}{\partial \tilde{N}}. \end{cases} \tag{1.22}$$

There are other variations of the Lotka–Volterra models and they also have a Poisson structure. (E.g., in [5] a three dimensional Lotka–Volterra model has been investigated.) We note that the Lotka–Volterra models can be successfully applied to the description of the human-resource interactions. This model can be considered to be an advanced Malthusian model of population growth. The predator–prey systems can be considered as follows: the human population is the predator and the resource is the prey. Based on this approach, several special ecological problems can be analysed, like the Easter Island collapse [10].

There are several geometric properties of such systems. One of them is the following. The solutions of the system lie on a closed curve [8], which means that the quantity of the prey and predator populations has periodic oscillation. This property is very basic for these phenomena, therefore in the construction of the discrete models to (1.17), it is important to use discretization methods for the system, that preserves this qualitative behaviour. Let

$$\omega_\tau = \{t_n = n\tau, \; n = 0, 1, \dots\} \tag{1.23}$$

where the mesh-size $\tau > 0$ is some given value. In the sequel P_n and N_n denote the approximation to the exact solution of the system at time t_n.

We apply some classical numerical one-step methods to the Lotka–Volterra system (1.17) and investigate their properties. The explicit Euler method results in the discrete model

$$N_{n+1} = N_n + \tau N_n(a - bP_n),$$
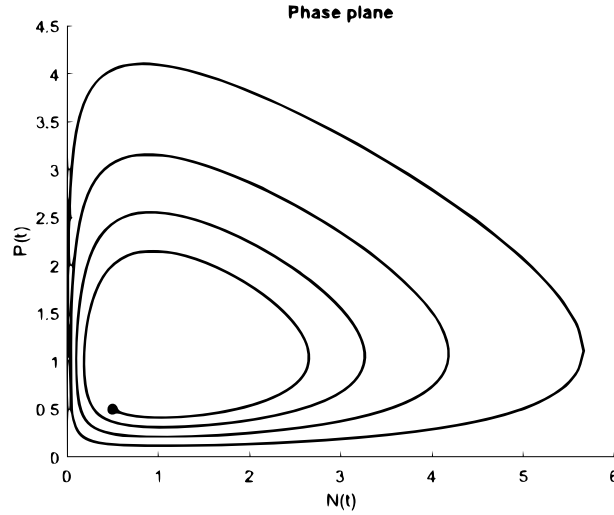$$P_{n+1} = P_n + \tau P_n(cN_n - d). \tag{1.24}$$

Figure 1.1: The numerical solution of the Lotka–Volterra system with the explicit Euler method, with $a = b = 1$, $c = d = 0.5$, $N_0 = P_0 = 0.5$ and $\tau = 0.1$.

The use of the implicit Euler method results in the model

$$N_{n+1} = N_n + \tau N_{n+1}(a - bP_{n+1}),$$
$$P_{n+1} = P_n + \tau P_{n+1}(cN_{n+1} - d). \tag{1.25}$$

Figure 1.1 and 1.2 suggest that the above methods do not preserve the geometric property, since the numerical solution spirals inwards or outwards, whereas the exact solution should lie on a closed curve.

In the following we define the preservation property of the numerical solution. Let Φ_τ represent the mapping of the one-step numerical method

$$\Phi_\tau : y_n \rightarrow y_{n+1} \tag{1.26}$$

which, by the analogy with (1.5), we call numerical flow.

Definition 1.16. A numerical method is called symplectic if the one-step map Φ_τ is symplectic whenever the method is applied to a smooth Hamiltonian system, i.e.,

$$\left(\Phi_\tau'(N_n, P_n)\right)^T J \left(\Phi_\tau'(N_n, P_n)\right) = J \tag{1.27}$$

is satisfied.

Definition 1.17. A numerical method is called a Poisson integrator if the numerical flow Φ_τ is a Poisson map, i.e., (1.16) holds.
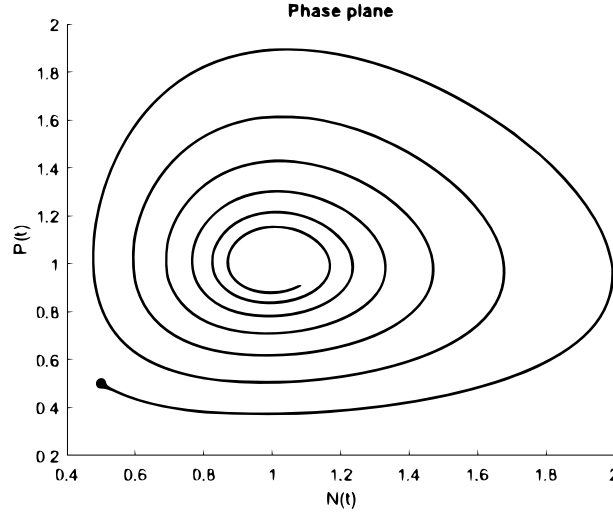
Figure 1.2: The numerical solution of the Lotka–Volterra system with the implicit Euler method, with $a = b = c = d = 1$, $N_0 = P_0 = 0.5$ and $\tau = 0.1$.

Hence, we have the following statements.

Theorem 1.18. *The explicit Euler and implicit Euler methods are neither symplectic nor Poisson integrators.*

Proof. In the following we denote by p^n and q^n the approximations of the unknown functions $N(t)$ and $P(t)$ at the time $t = t_n$, i.e. $N_n = p^n$ and $P_n = q^n$, respectively. Applying the explicit Euler method to the Hamiltonian system, we get the following one-step discrete model:

$$\begin{cases} p_{n+1} = p_n - \tau \dfrac{\partial H}{\partial q}(p_n, q_n) \\ q_{n+1} = q_n + \tau \dfrac{\partial H}{\partial p}(p_n, q_n). \end{cases} \tag{1.28}$$

Therefore,

$$\begin{cases} \dfrac{\partial p_{n+1}}{\partial p_n} = 1 - \tau \dfrac{\partial^2 H}{\partial q \partial p}(p_n, q_n) \\ \dfrac{\partial p_{n+1}}{\partial q_n} = -\tau \dfrac{\partial^2 H}{\partial q \partial q}(p_n, q_n) \\ \dfrac{\partial q_{n+1}}{\partial p_n} = \tau \dfrac{\partial^2 H}{\partial p \partial p}(p_n, q_n) \\ \dfrac{\partial q_{n+1}}{\partial q_n} = 1 + \tau \dfrac{\partial^2 H}{\partial p \partial q}(p_n, q_n). \end{cases} \tag{1.29}$$

From (1.29) by a simple calculation one can check that

$$(\Phi'_\tau(p_n, q_n))^T J (\Phi'_\tau(p_n, q_n)) \neq J, \tag{1.30}$$

which means that the explicit Euler method is not a symplectic integrator.
Applying the implicit Euler method to a Hamiltonian system, we get the following one-step numerical method:

$$\begin{cases} p_{n+1} = p_n - \tau \dfrac{\partial H}{\partial q}(p_{n+1}, q_{n+1}) \\ q_{n+1} = q_n + \tau \dfrac{\partial H}{\partial p}(p_{n+1}, q_{n+1}). \end{cases} \tag{1.31}$$

We differentiate the above relation with respect to p_n and q_n

$$\begin{cases} \dfrac{\partial p_{n+1}}{\partial p_n} = 1 - \tau \dfrac{\partial^2 H(p_{n+1}, q_{n+1})}{\partial p \partial q} \dfrac{\partial p_{n+1}}{\partial p_n} - \tau \dfrac{\partial^2 H(p_{n+1}, q_{n+1})}{\partial q \partial q} \dfrac{\partial q_{n+1}}{\partial p_n} \\[2mm] \dfrac{\partial p_{n+1}}{\partial q_n} = -\tau \dfrac{\partial^2 H(p_{n+1}, q_{n+1})}{\partial p \partial q} \dfrac{\partial p_{n+1}}{\partial p_n} - \tau \dfrac{\partial^2 H(p_{n+1}, q_{n+1})}{\partial q \partial q} \dfrac{\partial q_{n+1}}{\partial q_n} \\[2mm] \dfrac{\partial q_{n+1}}{\partial p_n} = \tau \dfrac{\partial^2 H(p_{n+1}, q_{n+1})}{\partial p \partial p} \dfrac{\partial p_{n+1}}{\partial p_n} + \tau \dfrac{\partial^2 H(p_{n+1}, q_{n+1})}{\partial q \partial q} \dfrac{\partial q_{n+1}}{\partial p_n} \\[2mm] \dfrac{\partial q_{n+1}}{\partial q_n} = 1 + \tau \dfrac{\partial^2 H(p_{n+1}, q_{n+1})}{\partial p \partial p} \dfrac{\partial p_{n+1}}{\partial p_n} + \tau \dfrac{\partial^2 H(p_{n+1}, q_{n+1})}{\partial p \partial q} \dfrac{\partial q_{n+1}}{\partial q_n}, \end{cases} \tag{1.32}$$

then the we get again

$$(\Phi'_\tau(p_n, q_n))^T J (\Phi'_\tau(p_n, q_n)) \neq J, \tag{1.33}$$

which means that the implicit Euler method is not a symplectic integrator.

Similarly it can be seen that the explicit and implicit Euler methods are not Poisson maps [4, 7]. □

Let us use an explicit-implicit method as follows:

$$\begin{aligned} N_{n+1} &= N_n + \tau N_{n+1}(a - bP_n), \\ P_{n+1} &= P_n + \tau P_n(cN_{n+1} - d). \end{aligned} \tag{1.34}$$

Figure 1.3 shows the numerical solution of the Lotka–Volterra system with the scheme (1.34). In this case the numerical result stays on a closed curve.
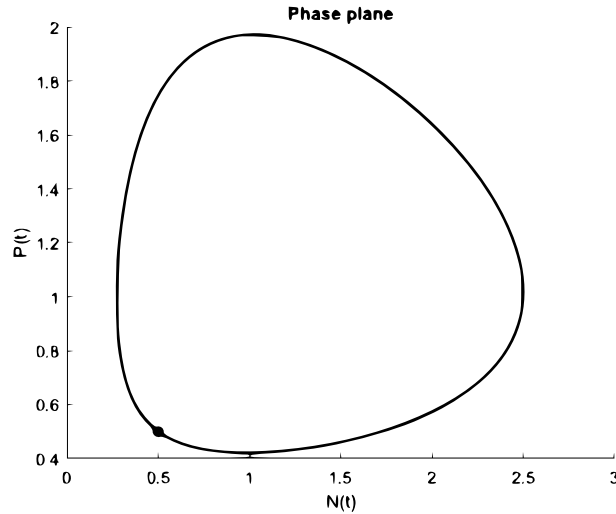

Figure 1.3: The numerical solution of the Lotka–Volterra system with the symplectic Euler method, with $a = 0.5$, $b = 1$, $c = 0.5$, $d = 1$, $N_0 = P_0 = 0.5$ and $\tau = 0.1$.

Theorem 1.19. *The numerical method* (1.34) *is a symplectic integrator for the transformed Lotka–Volterra system.*

Proof. We apply the above numerical method for the transformed Lotka–Volterra system (1.22) in the following form:

$$\begin{cases} N_{n+1} = N_n + \tau(-be^{P_n} + a) \\ P_{n+1} = P_n + \tau(ce^{N_{n+1}} - d) = P_n + \tau(e^{N_n + \tau(-be^{P_n} + a)} - d). \end{cases} \tag{1.35}$$

Differentiating these expressions with respect to N_n and P_n, we get

$$\begin{cases} \dfrac{\partial N_{n+1}}{\partial N_n} = 1 \\[2mm] \dfrac{\partial N_{n+1}}{\partial P_n} = -be^{P_n} \\[2mm] \dfrac{\partial P_{n+1}}{\partial N_n} = \tau e^{N_n + \tau(-be^{P_n} + a)} \\[2mm] \dfrac{\partial P_{n+1}}{\partial P_n} = 1 - be^{P_n} \tau e^{N_n + \tau(-be^{P_n} + a)}. \end{cases} \tag{1.36}$$

Hence,

$$\left(\Phi'_\tau(p_n, q_n)\right)^T J \left(\Phi'_\tau(p_n, q_n)\right) = J, \tag{1.37}$$

that means the numerical method is a symplectic integrator for the transformed Lotka–Volterra system. We call this method symplectic Euler method [4]. □

Theorem 1.20. *The symplectic Euler numerical method is a Poisson integrator for the Lotka–Volterra system* (1.17).

Proof. From the numerical model (1.34) using some simple calculation, we get

$$\left(\Phi'_\tau(N_n, P_n)\right)^T B(N_n, P_n)\left(\Phi'_\tau(N_n, P_n)\right) = B(N_{n+1}, P_{n+1}) \tag{1.38}$$

with $B(N_n, P_n)$ given in (1.20) and therefore, the method is a Poisson integrator. □

The symplectic Euler method, which was analysed in [4, 7], is a Poisson integrator and also symplectic for the Lotka–Volterra system. This is the reason why it gives good numerical results. In the next section we combine these methods with the operator splitting method and investigate the geometric properties.

2 Operator splitting methods for the Lotka–Volterra system

The operator splitting method is a powerful tool to lead the time dependent problems to a sequence of simpler sub-problems. This method separates the original equation into two or more parts over a time step, separately computes the solution to each part, and then combines the two or more separate solutions to form an approximation to the solution of the original differential equation. (The generalization for more sub-operators is straightforward, see [3]). We consider the following Cauchy problem

$$\begin{cases} \dfrac{dw}{dt} = \mathcal{A}(w(t)) + \mathcal{B}(w(t)), & 0 < t \leq T < \infty \\ w(0) = w_0, \end{cases} \tag{2.1}$$

where $w_0 \in \mathbb{R}^d$ is a given vector and the unknown function is $w : [0, T] \rightarrow \mathbb{R}^d$. We define a sequence of meshes on the solution domain, with the mesh size $\tau = \frac{M}{T}$. We replace the Cauchy problem (2.1) on the above defined M sub-intervals with the following modified Cauchy problems for each $n = 1, 2, \ldots, M$

$$\begin{cases} \dfrac{dw_1^n}{dt}(t) = \mathcal{A}(w_1^n(t)), & (n-1)\tau < t \leq n\tau, \\ w_1^n((n-1)\tau) = w_{sp}^n((n-1)\tau), \end{cases} \tag{2.2}$$

and

$$\begin{cases} \dfrac{dw_2^n}{dt}(t) = \mathcal{B}(w_2^n(t)), & (n-1)\tau < t \leq n\tau, \\ w_2^n((n-1)\tau) = w_1^n(n\tau). \end{cases} \tag{2.3}$$

Here $w_{sp}^0(0) = w_0$, and the function $w_{sp}^n(n\tau) = w_2^M(n\tau)$, defined at the points $t_n = n\tau$, $(n = 0, 1, \ldots, M)$ is called splitting solution of the Cauchy problem (2.1). We apply the operator splitting method to the Lotka–Volterra system (1.17) in the following way. Let

$$\begin{aligned} V_1(N_1, P_1) &= -a \ln P_1 - d \ln N_1, \\ V_2(N_2, P_2) &= bP_2 + cN_2 \end{aligned} \tag{2.4}$$

a resolution of the function V. In this case the splitting method leads to the following problems on the interval $(n-1)\tau < t \leq n\tau$ for each $n = 1, 2, \ldots, M$:

$$\begin{cases} \dfrac{dN_1^n(t)}{dt} = aN_1^n(t), & N_1^n(t_{n-1}) = N_{sp}^{n-1} \\ \dfrac{dP_1^n(t)}{dt} = -dP_1^n(t), & P_1^n(t_{n-1}) = P_{sp}^{n-1} \end{cases} \tag{2.5}$$

and

$$\begin{cases} \dfrac{dN_2^n(t)}{dt} = -bN_2^n(t)P_2^n(t), & N_2^n(t_{n-1}) = N_1^n(t_n) \\ \dfrac{dP_2^n(t)}{dt} = cN_2^n(t)P_2^n(t), & P_2^n(t_{n-1}) = P_1^n(t_n). \end{cases} \tag{2.6}$$

(Here the upper index n refers to the time interval where the sub-problems are defined.) The above problems can be solved analytically. The first system consists of two separable equations with the exact solution

$$N_1^n(t) = N_{sp}^{n-1}e^{at} \quad \text{and} \quad P_1^n(t) = P_{sp}^{n-1}e^{-dt}. \tag{2.7}$$

From the second differential equation, we get

$$\frac{d}{dt}(cN_2^n + bP_2^n) = 0. \tag{2.8}$$

Therefore $cN_2^n + bP_2^n = K_0$ is constant, that leads to a Bernoulli-type differential equation. Hence,

$$N_{sp}^n = \frac{e^{a\tau}N_{sp}^{n-1}K_0}{e^{K_0 t}\left[K_0 - ce^{at} \cdot N_{sp}^{n-1}\right] + ce^{at}N_{sp}^{n-1}} \tag{2.9}$$

$$P_{sp}^n = \frac{1}{b}\left[K_0 - cN_{sp}^n\right], \tag{2.10}$$

where K_0 has the form

$$K_0 = ce^{at}N_{sp}^{n-1} + be^{-dt}P_{sp}^{n-1}. \tag{2.11}$$

The flow of the system is the following:

$$\Phi_t = \begin{bmatrix} \Phi_t^1(N_{sp}^{n-1}, P_{sp}^{n-1}) \\ \Phi_t^2(N_{sp}^{n-1}, P_{sp}^{n-1}) \end{bmatrix}, \tag{2.12}$$

where

$$\Phi_t^1(N_{sp}^{n-1}, P_{sp}^{n-1}) := N_{sp}^n \quad \text{and} \quad \Phi_t^2(N_{sp}^{n-1}, P_{sp}^{n-1}) := P_{sp}^n. \tag{2.13}$$

With some simple calculation we arrive at the relation

$$(\Phi_t'(N_{sp}^{n-1}, P_{sp}^{n-1}))^T B(N_{sp}^{n-1}, P_{sp}^{n-1})\Phi_t'(N_{sp}^{n-1}, P_{sp}^{n-1}) \neq B(N_{sp}^n, P_{sp}^n), \tag{2.14}$$

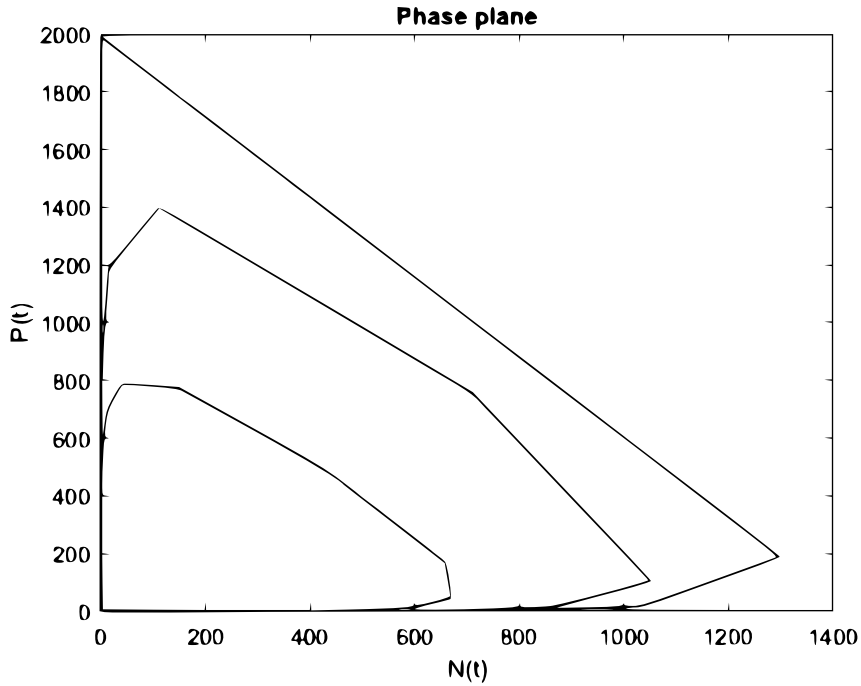which means the method is not a Poisson integrator.

Figure 2.1: The exact solution of system (2.5)–(2.6).

Figure 2.1 shows the exact solutions (2.9) of the systems (2.5)–(2.6). The results show that the solution of the discrete model does not preserve the cyclicity. This is the reason why we use numerical methods to solve both split sub-systems.

We have seen that the explicit Euler and implicit Euler methods in themselves do not preserve the above geometric property. In the sequel, we use the operator splitting method to solve the Lotka–Volterra system (1.17) and using numerical method to the sub-systems. Our expectations for this combined numerical method is that it preserves the geometric properties, namely the symplectic and Poisson structure. In the next sections we will investigate this problem.

2.1 Operator splitting method for a Hamiltonian system

We describe the numerical solution of a Hamiltonian system by using the operator splitting method with given initial conditions. First, we assume that $H(p,q) = H_1(p,q) + H_2(p,q)$ is some resolution of the Hamiltonian function. Then on each sub-interval $[t_n, t_{n+1}]$ the sequential splitting leads to two sub-problems as follows.

$$\begin{cases} \dfrac{dp_1}{dt} = -\dfrac{\partial H_1}{\partial q}(p_1(t), q_1(t)) \\ \dfrac{dq_1}{dt} = \dfrac{\partial H_1}{\partial p}(p_1(t), q_1(t)), \end{cases} \tag{2.15}$$

with $p_1(t_n) = p_{spl}^n$ and $q_1(t_n) = q_{spl}^n$, and

$$\begin{cases} \dfrac{dp_2}{dt} = -\dfrac{\partial H_2}{\partial q}(p_2(t), q_2(t)) \\ \dfrac{dq_2}{dt} = \dfrac{\partial H_2}{\partial p}(p_2(t), q_2(t)) \end{cases} \tag{2.16}$$

with $p_2(t_n) = p_1(t_{n+1})$ and $q_2(t_n) = q_1(t_{n+1})$. Then we set $p_{spl}^{n+1} = p_2(t_{n+1})$ and $q_{spl}^{n+1} = q_2(t_{n+1})$

We note that although both sub-systems (2.15) and (2.16) are Hamiltonian systems separately, but together they will not Hamiltonian systems anymore in general case.

We apply numerical methods with the step-size equal to the splitting step to these problems and investigate the symplecticity of their flow. We will use the notations p_i^n and q_i^n for the approximation of the functions $p_i(t)$ and $q_i(t)$ at the mesh-point $t = t_n$, respectively ($i = 1, 2$). We also use the following notations

$$\begin{aligned} A &= \frac{\partial^2 H_1}{\partial p^2}(p_1^n, q_1^n), & B &= \frac{\partial^2 H_1}{\partial q \partial p}(p_1^n, q_1^n), & C &= \frac{\partial^2 H_1}{\partial q^2}(p_1^n, q_1^n), \\ D &= \frac{\partial^2 H_2}{\partial p^2}(p_2^n, q_2^n), & E &= \frac{\partial^2 H_2}{\partial p \partial q}(p_2^n, q_2^n), & F &= \frac{\partial^2 H_2}{\partial q^2}(p_2^n, q_2^n). \end{aligned} \tag{2.17}$$

Then the following statement holds.

Theorem 2.1. *By use of the explicit Euler method with a step size equal to the splitting step size to solve the sub-systems (2.15) and (2.16), the combined numerical method is symplectic if the following conditions*

$$ACDF + ACE^2 - B^2 DF + B^2 E^2 - 2BCDE = 0$$
$$2ACE + 2CDE = 0 \tag{2.18}$$
$$AC - B^2 + DF - E^2 = 0$$

are satisfied.

Proof. Applying the explicit Euler method to the sub-problem (2.15) we get

$$\begin{cases} p_1^{n+1} = p_1^n - \tau \dfrac{\partial H_1}{\partial q}(p_1^n, q_1^n) \\ q_1^{n+1} = q_1^n + \tau \dfrac{\partial H_1}{\partial p}(p_1^n, q_1^n). \end{cases} \tag{2.19}$$

Similarly, the application of the explicit Euler method to the sub-problem (2.16) results in the relation

$$
\begin{cases}
p_2^{n+1} = p_2^n - \tau \dfrac{\partial H_2}{\partial q}(p_2^n, q_2^n) = p_1^{n+1} - \tau \dfrac{\partial H_2}{\partial q}(p_1^{n+1}, q_1^{n+1}) \\[2mm]
q_2^{n+1} = q_2^n + \tau \dfrac{\partial H_2}{\partial p}(p_2^n, q_2^n) = q_1^{n+1} + \tau \dfrac{\partial H_2}{\partial p}(p_1^{n+1}, q_1^{n+1}).
\end{cases}
\tag{2.20}
$$

For simplicity, we use the notation p^n and q^n for the approximation of the split solution at the mesh-point $t = t_n$. Then, the schemes (2.19) and (2.20) together yield the following one-step method

$$
\begin{cases}
p^{n+1} = p^n - \tau \dfrac{\partial H_2(p_1^{n+1}, q_1^{n+1})}{\partial q} \\[3mm]
q^{n+1} = q^n + \tau \dfrac{\partial H_2(p_1^{n+1}, q_1^{n+1})}{\partial p},
\end{cases}
\tag{2.21}
$$

where p_1^{n+1} and q_1^{n+1} are defined from (2.19) as follows

$$
\begin{cases}
p_1^{n+1} = p^n - \tau \dfrac{\partial H_1}{\partial q}(p^n, q^n) \\[3mm]
q_1^{n+1} = q^n + \tau \dfrac{\partial H_1}{\partial p}(p^n, q^n).
\end{cases}
\tag{2.22}
$$

We differentiate these expressions with respect to p and q. Then, according to the chain rule and the notations (2.17), we have

$$
\begin{aligned}
\frac{\partial p^{n+1}}{\partial p^n} &= \frac{\partial p_1^{n+1}}{\partial p^n} - \tau \frac{\partial H_2}{\partial p \partial q} \frac{\partial p_1^{n+1}}{\partial p^n} - \tau \frac{\partial H_2}{\partial^2 q} \frac{\partial q_1^{n+1}}{\partial p^n} = 1 - \tau B - \tau E(1 - \tau B) - \tau^2 F A \\[2mm]
\frac{\partial p^{n+1}}{\partial q^n} &= \frac{\partial p_1^{n+1}}{\partial p^n} - \tau \frac{\partial^2 H_2}{\partial q^2} \frac{\partial q_1^{n+1}}{\partial p^n} - \tau \frac{\partial^2 H_2}{\partial p \partial q} \frac{\partial p_1^{n+1}}{\partial p^n} = -\tau C - \tau^2 C E - \tau F(1 + \tau B) \\[2mm]
\frac{\partial q^{n+1}}{\partial p^n} &= \frac{\partial q_1^{n+1}}{\partial p^n} + \tau \frac{\partial^2 H_2}{\partial p^2} \frac{\partial p_1^{n+1}}{\partial p^n} + \tau \frac{\partial^2 H_2}{\partial p \partial q} \frac{\partial q_1^{n+1}}{\partial p^n} = \tau A + \tau D(1 - \tau B) + \tau^2 A \\[2mm]
\frac{\partial q^{n+1}}{\partial q^n} &= \frac{\partial q_1^{n+1}}{\partial q^n} + \tau \frac{\partial^2 H_2}{\partial p^2} \frac{\partial p_1^{n+1}}{\partial q^n} + \tau \frac{\partial^2 H_2}{\partial p \partial q} \frac{\partial q_1^{n+1}}{\partial q^n} = 1 + \tau B - \tau^2 C D + \tau E(1 + \tau B).
\end{aligned}
\tag{2.23}
$$

Hence, computing the matrix product $(\Phi'_\tau(p_n, q_n))^T J (\Phi'_\tau(p_n, q_n))$ we obtain the sufficient conditions (2.18) for the symplecticity. $\qquad\square$

This statement shows that the explicit Euler method in itself is not a symplectic integrator, but when we use the operator splitting method with some suitable resolution of the Hamiltonian function, with such a distribution the method can be symplectic.

The conditions (2.18) are usually very restricitive. Therefore our aim is to relax these conditions by choosing other numerical methods for solving the split sub-problems. In the following we investigate the combination of the symplectic Euler method and the non-symplectic explicit Euler method. We split the Hamiltonian function into two parts and solve these two sub-systems with the above numerical methods. Let $H(p, q) = H_1(p, q) + H_2(p, q)$ and we solve the first problem with the explicit Euler method

$$
\begin{cases}
p_1^{n+1} = p_1^n - \tau \dfrac{\partial H_1(p_1^n, q_1^n)}{\partial q} \\[3mm]
q_1^{n+1} = q_1^n + \tau \dfrac{\partial H_1(p_1^n, q_1^n)}{\partial p},
\end{cases}
\tag{2.24}
$$

then to the second problem we use the symplectic Euler method

$$\begin{cases} p_2^{n+1} = p_2^n - \tau \dfrac{\partial H_2(p_2^{n+1}, q_2^n)}{\partial q}, \\[3mm] q_2^{n+1} = q_2^n + \tau \dfrac{\partial H_2(p_2^{n+1}, q_2^n)}{\partial p}. \end{cases} \tag{2.25}$$

Theorem 2.2. *The combination of the explicit Euler and symplectic Euler method* (2.24)–(2.25) *results in a symplectic numerical method if the condition*

$$A \cdot B - C = 0 \tag{2.26}$$

is satisfied.

Proof. In the same way, as before to the split porblem (2.15)–(2.16), for this approach the combined method of the explicit and symplectic Euler method can be written as a one-step numerical method, as follows

$$\begin{cases} p^{n+1} = p^n - \tau \dfrac{\partial H_2(p^{n+1}, q^n)}{\partial q} \\[3mm] q^{n+1} = q^n + \tau \dfrac{\partial H_2(p^{n+1}, q^n)}{\partial p}, \end{cases} \tag{2.27}$$

where $p^{n+1} = p_2^{n+1}$, $q^{n+1} = q_2^{n+1}$ and $q^n = q_1^{n+1}$. We differentiate these expressions with respect to p^n, q^n

$$\begin{aligned} \frac{\partial p^{n+1}}{\partial p^n} &= 1 - \tau \frac{\partial^2 H_1(p_1^n, q_1^n)}{\partial p_1 \partial q_1} - \tau \frac{\partial^2 H_2(p^{n+1}, q^n)}{\partial p \partial q} \cdot \frac{\partial p^{n+1}}{\partial p^n} \\ &\quad - \tau^2 \frac{\partial^2 H_2(p^{n+1}, q^n)}{\partial q \partial q} \cdot \frac{\partial^2 H_1(p_1^n, q_1^n)}{\partial p_1 \partial p_1}, \\ \frac{\partial p^{n+1}}{\partial q^n} &= -\tau \frac{\partial^2 H_1(p_1^n, q_1^n)}{\partial q_1 \partial q_1} - \tau \frac{\partial^2 H_2(p^{n+1}, q^n)}{\partial p \partial q} \cdot \frac{\partial p^{n+1}}{\partial q^n} \\ &\quad - \tau \frac{\partial^2 H_2(p^{n+1}, q^n)}{\partial q \partial q} \cdot \left(1 + \tau \frac{\partial^2 H_1(p_1^n, q_1^n)}{\partial p_1 \partial q_1}\right), \\ \frac{\partial q^{n+1}}{\partial p^n} &= \tau \frac{\partial^2 H_1(p_1^n, q_1^n)}{\partial p_1 \partial p_1} + \tau \frac{\partial^2 H_2(p^{n+1}, q^n)}{\partial p \partial p} \cdot \frac{\partial p^{n+1}}{\partial p^n} \\ &\quad + \tau^2 \frac{\partial^2 H_2(p^{n+1}, q^n)}{\partial p \partial q} \cdot \frac{\partial^2 H_1(p_1^n, q_1^n)}{\partial p_1 \partial p_1}, \\ \frac{\partial q^{n+1}}{\partial q^n} &= 1 + \tau \frac{\partial^2 H_1(p_1^n, q_1^n)}{\partial p_1 \partial q_1} + \tau \frac{\partial^2 H_2(p^{n+1}, q^n)}{\partial p \partial p} \cdot \frac{\partial p^{n+1}}{\partial q^n} \\ &\quad + \tau \frac{\partial^2 H_2(p^{n+1}, q^n)}{\partial p \partial q} \cdot \left(1 + \tau \frac{\partial^2 H_1(p_1^n, q_1^n)}{\partial p_1 \partial q_1}\right). \end{aligned} \tag{2.28}$$

Hence,

$$(\Phi_\tau'(p_n, q_n))^T J (\Phi_\tau'(p_n, q_n)) = \begin{pmatrix} 0 & A \cdot B - C + 1 \\ -A \cdot B + C - 1 & 0 \end{pmatrix}.$$

Then, by the definition, the numerical method is symplectic if the condition

$$A \cdot B - C = 0 \tag{2.29}$$

is satisfied.   □

If we apply these results to the Lotka–Volterra system and choose

$$H_1 = -a\tilde{P}_1 - d\tilde{N}_1 \quad \text{and} \quad H_2 = be^{\tilde{P}_2} + ce^{\tilde{N}_2}, \tag{2.30}$$

the condition of Theorem 2.2 is satisfied. In this case the operator splitting has the following biological meaning: the corresponding system has been divided into two terms. The function H_1 shows the growth rate and H_2 contains the interaction terms. Figure 2(a) shows the numerical solution with the explicit Euler and symplectic Euler method, when the parameters are $a = 1, b = 0.6, c = 0.5, d = 1$. The solution lies on a closed curve.
We fix these parameters and use the explicit Euler method to solve both systems. We can see that in Figure 2(b). In this case the numerical solution spirals outwards.
Let us use the explicit Euler method with another symplectic Euler method and a resolution of the Hamiltonian which does not satisfy the condition of Theorem 2.2, namely,

$$H_1(\tilde{N}_1, \tilde{P}_1) = be^{\tilde{P}_1} + ce^{\tilde{N}_1}, \tag{2.31}$$

$$H_2(\tilde{N}_2, \tilde{P}_2) = -a\tilde{P}_2 - d\tilde{N}_2. \tag{2.32}$$

Then the numerical method is not symplectic, see Figure 2(c) that shows these cases.

The results show that the adequate combination of numerical methods and splitting methods are useful to preserve the symplectic structure of the numerical solution. As we have seen, the symplecticity depends on the numerical method and the resolution of the Hamiltonian system, too.

3 Operator splitting method for a Poisson system

We describe the numerical method of the system (1.17) by using the operator splitting method of the form

$$\begin{cases} \dfrac{dN}{dt} = -NP \cdot \dfrac{\partial V(N,P)}{\partial P}, & N(0) = N_0 \\ \dfrac{dP}{dt} = NP \cdot \dfrac{\partial V(N,P)}{\partial N}, & P(0) = P_0. \end{cases} \tag{3.1}$$

We investigate the combination of two implicit methods, namely, the implicit Euler method and the symplectic Euler method which results in the sub-problems

$$\begin{cases} \dfrac{dN_1^{n+1}}{dt} = N_1^n - \tau N_1^{n+1} P_1^{n+1} \cdot \dfrac{\partial V_1(N_1^{n+1} P_1^{n+1})}{\partial P_1}, \\ \dfrac{dP_1^{n+1}}{dt} = P_1^n + \tau N_1^{n+1} P_1^{n+1} \cdot \dfrac{\partial V_1(N_1^{n+1}, P_1^{n+1})}{\partial N_1}, \end{cases} \tag{3.2}$$

$$\begin{cases} \dfrac{dN_2^{n+1}}{dt} = N_2^n - \tau N_2^{n+1} P_2^n \cdot \dfrac{\partial V_2(N_2^{n+1}, P_2^n)}{\partial P_2} \\ \dfrac{dP_2^{n+1}}{dt} = P_2^n + \tau N_2^{n+1} P_2^n \cdot \dfrac{\partial V_2(N_2^{n+1}, P_2^n)}{\partial N_2}. \end{cases} \tag{3.3}$$

Theorem 3.1. *If we use the combination of the implicit Euler and symplectic Euler method to solve the system (1.17) and the resolution (2.4), then the numerical method is a Poisson integrator.*
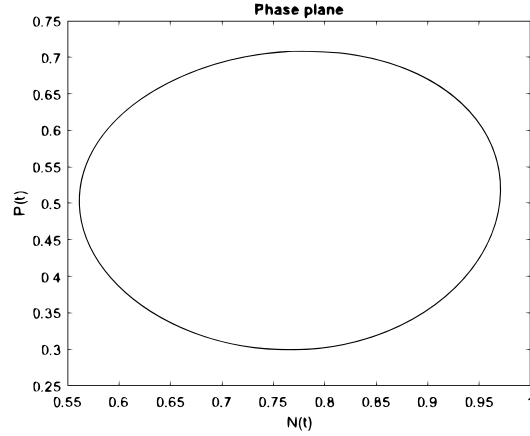
(a) Numerical solution with the explicit Euler and symplectic Euler method.
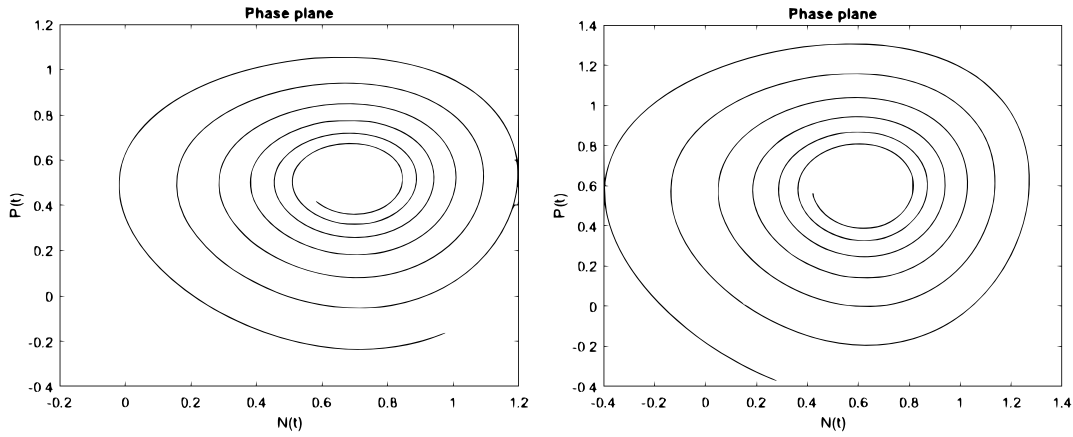
(b) Numerical solution with the explicit Euler method.

(c) Numerical solution with the explicit Euler and symplectic Euler method with another resolution of the Hamiltonian system.

Figure 2.2: The numerical solution with the operator splitting method.

Proof. In this case the modified Cauchy problems are the following:

$$N_1^{n+1} = \frac{N_1^n}{1 - \tau a}, \qquad N_1^n = N_{sp}^n,$$

$$P_1^{n+1} = \frac{P_1^n}{1 + \tau d}, \qquad P_1^n = P_{sp}^n, \tag{3.4}$$

and

$$N_2^{n+1} = \frac{N_2^n}{1 + b\tau P_2^n}, \qquad N_2^n = N_1^{n+1},$$

$$P_2^{n+1} = P_2^n + \tau c N_2^{n+1} P_2^n, \qquad P_2^n = P_1^{n+1}. \tag{3.5}$$

Hence,

$$\begin{cases} N_2^{n+1} = \dfrac{(1 + \tau d)N_1^n}{(1 - \tau a)(1 + \tau d + b\tau P_1^n)} \\[2ex] P_2^{n+1} = (1 + \tau c N_1^{n+1}) \cdot \dfrac{P_1^n}{1 + \tau d}. \end{cases} \tag{3.6}$$

Applying operator splitting and (3.6), we obtain

$$\begin{cases} N^{n+1} = \dfrac{(1+\tau d)N^n}{(1-\tau a)(1+\tau d + b\tau P^n)} \\ P^{n+1} = (1+\tau c N^{n+1}) \cdot \dfrac{P^n}{1+\tau d} \end{cases} \tag{3.7}$$

and differentiating these expressions with respect to N^n and P^n, we obtain

$$\begin{aligned} \frac{\partial N^{n+1}}{\partial N^n} &= \frac{1+\tau d}{(1-\tau a)(1+\tau d + b\tau P^n)} \\ \frac{\partial N^{n+1}}{\partial P^n} &= \frac{-b\tau(1+\tau d)N^n}{(1-\tau d)(1+\tau d + b\tau P^n)^2} \\ \frac{\partial P^{n+1}}{\partial N^n} &= 0 \\ \frac{\partial P^{n+1}}{\partial P^n} &= \frac{1+\tau c N^{n+1}}{1+\tau d}. \end{aligned} \tag{3.8}$$

Therefore, the following condition holds:

$$(\Phi_\tau'(N_n, P_n))^T B(N_n, P_n) \Phi_\tau'(N_n, P_n) = B(N_{n+1}, P_{n+1}) \tag{3.9}$$

so the method is a Poisson integrator. $\qquad\square$

If we choose $V_1 = -a \ln P - d \ln N$ and $V_2 = bP + cN$, the numerical method is a Poisson integrator. Figure 3.1 shows the numerical solution with the explicit Euler and symplectic Euler method, when the parameters are $a = 0.2, b = c = 0.5$ and $d = 0.3$. The solution lies on a closed curve. We fix these parameters and use the implicit Euler and explicit Euler method
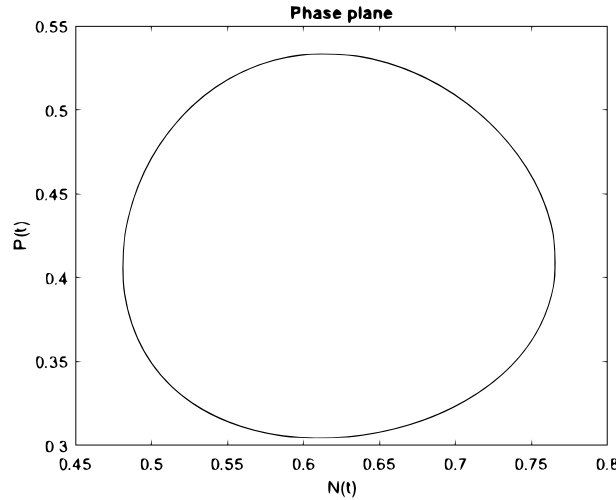

Figure 3.1: Numerical solution with the implicit Euler and symplectic Euler method.

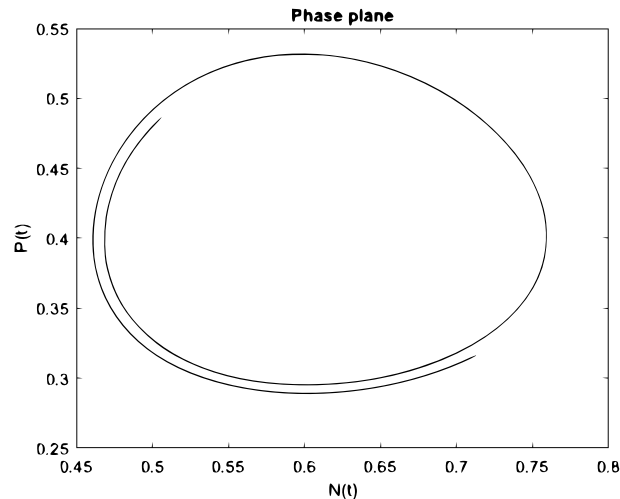to solve the systems. In this case Figure 3.2 shows that the numerical solution spirals outward.

Figure 3.2: Numerical solution with the implicit Euler and explicit Euler method.

4   Summary

It is essential to use numerical methods, that preserve geometric structures when modelling biological or physics phenomena. These methods enable us to construct mathematical models that are much closer to the real-life systems. In this article we have investigated Hamiltonian systems and Poisson systems and the geometric properties of their flow.

   We have analysed the Lotka–Volterra predator–prey system, which is a pair of ordinary differential equations. The Lotka–Volterra system has a certain geometric structure: the solutions lie on a closed curve. We used the operator splitting method and the combination of the classical and simplest one-step numerical methods: explicit and implicit Euler method and the symplectic Euler method to solve the Lotka–Volterra equation system. We have investigated the geometric properties of the flows of the numerical methods. We have seen that it is important to carefully choose the appropriate operator splitting method and numerical methods when solving Hamiltonian and Poisson systems.

Acknowledgements

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