Numerical integration of ODEs while preserving all polynomial first integrals

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Abstract

We present a novel method for solving ordinary differential equations (ODEs) while preserving all polynomial first integrals. The method is essentially a symplectic Runge-Kutta method applied to a reformulated version of the ODE under study and is illustrated through a number of examples including Hamiltonian ODEs, a Nambu system and the Toda Lattice. When applied to certain Hamiltonian ODEs, the proposed method yields the averaged vector field method as a special case.

1 Introduction

In this paper, we are concerned with the numerical solution of autonomous ODEs in $n$ dimensions

$$\dot{x} = f(x), \quad x \in \mathbb{R}^n,$$

that possess the functions $H_i(x)$ for $i = 1, ..., m < n$ satisfying $\dot{H}_i(x) = f(x) \cdot \nabla H_i(x) = 0$, where the dot denotes $\frac{d}{dt}$. If such functions exist, they are called first integrals of (1). The preservation of first integrals under numerical methods is an important property for the method to inherit when performing long-term simulations of dynamical systems [1]. Hamiltonian systems, for instance, are an important class of ODEs that govern many physical phenomena and have subsequently been the subject of many influential studies. Many well designed energy-preserving methods have therefore been proposed for solving such systems, for example, discrete gradient methods [2,3], Hamiltonian boundary value methods [4] and Runge-Kutta type methods [5–7]. In particular, the energy-preserving averaged vector field method, which was first introduced in [8], has been the building block of many interesting methods for such canonical Hamiltonian ODEs [9,10]. The study of energy-preserving numerical methods for ODEs often also serves as inspiration for many energy-preserving methods for Hamiltonian PDEs including discrete variational methods [11,12], averaged vector field methods [13,14], continuous Runge-Kutta type methods [15] and fast linearly implicit methods based on polarization [16] or discrete gradients [17]. Another successful
energy-preserving method for Hamiltonian PDEs is the scalar auxiliary variable approach \[18\], \[19\]. However, many dynamical systems possess \textit{multiple} first integrals such as Lie-Poisson systems, lattice equations, Nambu systems and many other integrable systems. As it is desirable for numerical simulations to inherit as many physical properties of the exact solution as possible, numerical methods for preserving multiple first integrals have been considered. Although this is a much more difficult task than preserving a single first integral, many successful methods have been constructed in the past that utilize projection \[20\], \[21\] and/or discrete gradients \[3\], \[22\], which is a form of projection \[23\]. However, as noted in \[24\], projection is somewhat of a last resort as it destroys other properties of the solution such as the affine covariance and may not give good long time behavior. Other methods for preserving multiple first integrals that are worth mentioning are the line integral methods \[25\], \[26\].

Here, we present a novel numerical method that preserves all polynomial integrals \(H_i(x)\) of an ODE of the form (1). The method is simple and is essentially the midpoint rule, or a higher order symplectic Runge-Kutta method, but applied to a reformulated version of the ODE under study in a higher dimensional phase space then projected exactly onto the original phase space. The method is therefore implicit, symmetric, of arbitrary order and roughly the same computational cost of an implicit Runge-Kutta method. Furthermore, when restricted to some canonical Hamiltonian ODEs our method yields the averaged vector field method as a special case.

The paper is organized as follows. We begin in section 2.1 by introducing a simplified version of the method for a quartic-Hamiltonian ODE. Here, we illustrate the core concept using an example of the planar quartic oscillator. Once this has been elucidated then extending the method to preserve polynomial integrals (i.e., of arbitrary degree), then multiple polynomial integrals follows straightforwardly. This is presented in sections 2.2 and 2.3 respectively. In section 2.4 we show how to develop higher-order methods and in section 2.5 we briefly discuss the connection between the proposed method and the averaged vector field method. Section 3 presents numerical examples of a Hamiltonian system, a Nambu system and the Toda lattice. Concluding remarks are given in section 4.

2 Integral-preserving numerical integration

2.1 Quartic-Hamiltonian ODEs

Let \(\mathbb{R}_d[x]\) be the class of polynomials of degree \(d\) in the variables \(x \in \mathbb{R}^n\). To introduce the method, we first focus our attention on an \(n\)-dimensional Hamiltonian ODE with a quartic Hamiltonian \(H(x) \in \mathbb{R}_4[x]\) for \(n\) even. Such an ODE takes the form

\[
\dot{x} = J \nabla H(x),
\]

where \(J = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}\), \(I\) is the identity matrix in \(n/2\) dimensions and \(\nabla\) is the gradient operator with respect to \(x\). We note that the forthcoming method is applicable to ODEs with non-constant symplectic structure and in odd dimension, i.e., when \(J = J(x)\).

To construct the integral preserving method, we start by introducing the quadratic auxiliary variables

\[ y_{i,j} = x_i x_j \quad \text{for} \quad j \leq i, \quad i = 1, ..., n \]
and define what will be referred to as a reduced-degree Hamiltonian \( \tilde{H}(x, y) \in \mathbb{R}_2[x, y] \) that is quadratic in the variables \( x \) and \( y \) and satisfies the consistency condition

\[
\tilde{H}(x, y(x)) = H(x).
\]

Here, with a slight abuse of notation, we have let \( y = (y_{1,1}, y_{1,2}, ..., y_{n,n-1}, y_{n,n})^T \in \mathbb{R}^m \) denote the \( m = n(n+1)/2 \) independent quadratic auxiliary variables and \( y(x) = (x_1x_1, x_1x_2, ..., x_nx_{n-1}, x_nx_n)^T \) (i.e., with the argument \( x \) written explicitly) denote the \( y \) variables as a function of the original phase space variables \( x \). Using the chain rule, the ODE in these new variables now reads

\[
\dot{x} = J \nabla \tilde{H}(x, y) = J \left( \frac{\partial}{\partial x} \tilde{H}(x, y) + \frac{\partial y(x)}{\partial x} \frac{\partial}{\partial y} \tilde{H}(x, y) \right) := f(x, y) \tag{3}
\]

\[
\dot{y} = \frac{\partial y(x)}{\partial x} f(x, y) := g(x, y)
\]

We will refer to \( f(x, y) \) as the reduced-degree vector field of \( f(x) \) with respect to \( \tilde{H}(x, y) \), which also satisfies the consistency condition \( f(x, y(x)) = f(x) \). Furthermore, we will refer to the collective ODE system (3) as the extended ODE. We now make some observations.

**Remark 1.** The extended ODE (3):

(a) is of the following skew gradient form for \( z = (x^T, y^T)^T \)

\[
\dot{z} = S(z) \nabla \tilde{H}(z), \quad S(z) = -S(z)^T = \begin{pmatrix} J & -\left( \frac{\partial y(x)}{\partial x} \right)^T J \\
\frac{\partial y(x)}{\partial x} J & \frac{\partial y(x)}{\partial x} J \frac{\partial y(x)}{\partial x}^T \end{pmatrix}.
\]

(b) has the reduced-degree Hamiltonian \( \tilde{H}(x, y) \) as first integral. This follows directly from (a).

(c) possesses the \( m \) additional quadric integrals

\[
H_{i,j}(x, y) = x_i x_j - y_{i,j}, \quad i = 1, ..., n, \quad j \leq i.
\]

This can be easily seen by differentiating with respect to \( t \)

\[
\dot{H}_{i,j} = \dot{x}_i x_j + \dot{x}_j x_i - \dot{y}_{i,j} = f_i(x, y)x_j + f_j(x, y)x_i - (f_i(x, y)x_j + f_j(x, y)x_i) = 0.
\]

(d) is solved by the solution of (2) with the initial conditions \( y_{i,j} \big|_{t=0} = x_i x_j \big|_{t=0} \).

Due to remark 1d, an integral-preserving method of the ODE (3) will yield an integral-preserving method of (2) as long as the outlined initial conditions \( y_{i,j} \big|_{t=0} = x_i x_j \big|_{t=0} \) are satisfied. Moreover, the \( m \) induced quadric integrals \( H_{i,j}(x, y) \) together with the reduced-degree Hamiltonian \( \tilde{H}(x, y) \) are quadratic, therefore any symplectic Runge-Kutta method (i.e., one with vanishing stability matrix [27]) will preserve all such integrals. However, numerically integrating the ODE (3) presents a significant drawback, namely that the phase space dimension has increased from \( n \) to \( n + m = n(n+3)/2 \). Due to the fact that \( m \) scales quadratically with \( n \) this quickly becomes computationally prohibitive for large \( n \) especially due to the fact all symplectic Runge-Kutta methods are implicit.
However, this issue can be circumvented as follows. First we implement the (symplectic) midpoint rule given by

\[
\frac{x' - x}{h} = f \left( \frac{x' + x}{2}, \frac{y' + y}{2} \right), \quad (4)
\]
\[
\frac{y' - y}{h} = g \left( \frac{x' + x}{2}, \frac{y' + y}{2} \right), \quad (5)
\]

where \(x' \approx x(h)\) denotes the solution of the midpoint rule from initial conditions \(x = x(0)\) and similarly for \(y\). Due to the fact that the midpoint rule preserves all quadratic invariants, we have preservation of the induced quadratic integrals \(H_{i,j}(x', y') = H_{i,j}(x, y)\), which is a linear equation for \(y'\) meaning it’s solution can be directly found in terms of \(x'\) and therefore avoiding the need to solve \((5)\). That is, by substituting \(y'_{i,j} = x'_i x'_j\) into \((4)\) we are left with an \(n\) dimensional implicit equation for \(x'\) as follows

\[
\frac{x' - x}{h} = f \left( \frac{x' + x}{2}, \frac{y(x') + y(x)}{2} \right). \quad (6)
\]

Doing so circumvents the issue of the increased phase space dimension, thus yielding an efficient method that preserves any quartic Hamiltonian. The method \((6)\) will be referred to as the reduced-degree midpoint method.

**Remark 2.** We observe that the reduced-degree midpoint method:

(a) possesses a B-series with respect to the extended ODE vector field.

(b) is affinely equivariant with respect to the variables \((x, y)\).

(c) is symmetric, that is, it is invariant under the transformation \(x \leftrightarrow x'\) and \(h \rightarrow -h\).

(d) is order two.

(e) is energy-preserving even for non-constant symplectic structure, i.e. when \(J = J(x)\) and for odd dimension.

These observations can be seen as follows. By letting \(z = (x^T, y^T)^T\) denote the \(n + m\) dependent variables and \(P_n = (I_n, 0_{n,m}) \in \mathbb{R}^{n \times (n+m)}\) the projection operator such that \(P_n z = x\), then the reduced-degree midpoint method \((6)\) is none other than \(P_n z'\), where \(z'\) is one step of the midpoint rule applied to the extended ODE, hence it shares the properties of the midpoint rule. The observations then follow from the fact that the midpoint method is an order-two, symmetric Runge-Kutta method. We also note that while the midpoint rule is symplectic, the reduced-degree midpoint rule is not due to the fact that the reformulating the ODE into its extended form destroys the symplectic structure of the original Hamiltonian ODE. Two interesting questions arise from this. The first is how does the B-series of the extended vector field relate to that of the original one; the second is how does the symplectic structure of \((2)\) relate to the numerical flow the extended ODEs. We will leave these topics for a future study.

Lastly, we note that the reduced-degree midpoint rule is not uniquely defined for all Hamiltonians. Consider, for example, \(H(x) = x_1^2 + x_2^2\). Then one clearly has some freedom in how to reduce the quartic term, for example, one could take linear combinations of such choices and set

\[
\tilde{H}(x, y) = x_1^2 + (\beta y_1, y_2, 2 + (1 - \beta)y_{1,2}^2),
\]
where $\beta \in \mathbb{R}$ is a free parameter. This allows for a family of methods to be constructed for certain Hamiltonians. We will now demonstrate our method with an example.

### 2.1.1 Example: The quartic oscillator

Consider the quartic oscillator with Hamiltonian

$$H(x_1, x_2) = \frac{1}{2} x_1^2 + \frac{1}{4} x_2^4 \in \mathbb{R}[x_1, x_2]$$

that corresponds to the ODE

$$\dot{x}_1 = -x_2^3, \quad \dot{x}_2 = x_1.$$ 

Now introduce the variable $y_{2,2} = x_2^2$ and define the following reduced-degree Hamiltonian

$$\tilde{H}(x_1, x_2, y_{2,2}) = \frac{1}{2} x_1^2 + \frac{1}{4} y_{2,2}^2 \in \mathbb{R}[x_1, x_2, y_{2,2}].$$

Note that this satisfies the consistency condition $\tilde{H}(x_1, x_2, x_2^2) = H(x_1, x_2)$. The corresponding extended ODE system for $x_1, x_2$ and $y_{2,2}$ (i.e., equation (3)) is therefore

$$\dot{x}_1 = -x_2 y_{2,2}, \quad \dot{x}_2 = x_1,$$ 

$$\dot{y}_{2,2} = 2x_1 x_2,$$  \hspace{0.5cm} where $y_{2,2}|_{t=0} = x_2^2|_{t=0}$,

to which we apply the midpoint rule (i.e., equations (4) and (5))

$$\frac{x'_1 - x_1}{h} = - \left( \frac{x'_2 + x_2}{2} \right) \left( \frac{y'_{2,2} + y_{2,2}}{2} \right),$$

$$\frac{x'_2 - x_2}{h} = \left( \frac{x'_1 + x_1}{2} \right),$$

$$\frac{y'_{2,2} - y_{2,2}}{h} = 2 \left( \frac{x'_1 + x_1}{2} \right) \left( \frac{x'_2 + x_2}{2} \right).$$

The ODE (7) possesses the integrals $\tilde{H}(x_1, x_2, y_{2,2})$ and $H_{2,2}(x_1, x_2, y_{2,2}) = y_{2,2} - x_2^2$, both of which are quadratic and are therefore preserved by the midpoint rule. This means $y'_{2,2} - x_2^2 = y_{2,2} - x_2^2$ and due to the fact that the initial conditions satisfy $y_{2,2} = x_2^2$, we have $y'_{2,2} = x_2^2$. Substituting this into equation (8) we derive the reduced-degree midpoint rule (i.e., equation (6))

$$\frac{x'_1 - x_1}{h} = - \left( \frac{x'_2 + x_2}{2} \right) \left( \frac{x'_2 + x_2^2}{2} \right),$$

$$\frac{x'_2 - x_2}{h} = \left( \frac{x'_1 + x_1}{2} \right),$$

which is equivalent to the midpoint rule applied to the extended system (8) projected onto the $x$ coordinates. This concept is depicted in figure 1. Here, the numerical solution using the midpoint rule applied to the three dimensional extended ODE (8) is given by the thick black line and
Figure 1: The numerical solution of the midpoint method applied to the 3 dimensional extended ODEs (thick black line), the reduced-degree midpoint method applied to the original 2 dimensional Hamiltonian ODE (dotted black line), the level sets of the original quartic Hamiltonian $H(x_1, x_2)$ (thin black lines) and the iso-surfaces of the reduced-degree Hamiltonian $\tilde{H}(x_1, x_2, y_{2,2})$ and the induced quadric integral $H_{2,2}(x_1, x_2, y_{2,2})$ (colored surfaces). The simulation uses the initial conditions $x_1(0) = 1$, $x_2(0) = 1$ and $y_{2,2}(0) = x_2(0)^2$. Note that the reduced-degree midpoint method is the projection of the midpoint method applied to the three dimensional extended ODEs onto the $x_1 - x_2$ plane, which coincides with a level set of the $H(x_1, x_2)$.

The reduced-degree midpoint rule \([9]\) is given by the dashed line and is confined to the $x_1 - x_2$ plane. The isosurfaces of the reduced-degree Hamiltonian $\tilde{H}(x_1, x_2, y_{2,2})$ and the induced integral $H_{2,2}(x_1, x_2, y_{2,2})$ are also displayed as colored surfaces. We see that the numerical flow of the midpoint rule \([8]\) is confined to the intersection of these two quadrics. Moreover, the numerical flow of the reduced-degree midpoint method is none other than the projection of this curve onto the $x_1 - x_2$ plane. This projection also coincides with the level set of the original quartic Hamiltonian $H(x_1, x_2)$ and hence is preserved by the reduced-degree midpoint method. Finally, we note that the method \([9]\) is identical to the averaged vector field method.

In the rest of the paper, we will show how to apply the reduced-degree midpoint method to develop: (1) methods that preserve polynomial integrals (i.e., of arbitrarily high degree); (2) methods that preserve multiple polynomial integrals; and (3) high-order methods that preserve multiple polynomial integrals.

2.2 Preservation of polynomial integrals

Consider an ODE of the form \([1]\). Then \([1]\) possesses an integral $H(x)$ if and only if it can be expressed in the following skew-gradient form \([28]\)

$$\dot{x} = S(x) \nabla H(x),$$

where $S(x) = -S(x)^T$ is a skew-symmetric matrix. We now focus on the case where $H(x) \in \mathbb{R}_d[x]$ is a polynomial integral of degree $d$ and show how to extend the reduced-degree midpoint rule to preserve such an integral.
Similarly to the previous section, we start by defining a quadratic reduced-degree integral \( \tilde{H}(x, y^{[1]}, \ldots, y^{[n_y]}) \in \mathbb{R}^2[x, y^{[1]}, \ldots, y^{[n_y]}] \) for \( n_y \geq \log_2(d) - 1 \) by introducing the change of variables inductively defined by \( y^{[0]}_i = x_i \) and \( y^{[k]}_{i,j} = y^{[k-1]}_i y^{[k-1]}_j \), where \( i \) is a multi-index. For example, \( y^{[1]}_{i,j} = x_i x_j \) and \( y^{[2]}_{i,j,k,l} = y^{[1]}_i y^{[1]}_j y^{[1]}_k y^{[1]}_l \), where the latter can be abbreviated using the multi-index notation by \( y^{[2]}_{i,j} = y^{[1]}_i y^{[1]}_j \).

Note that the degree of \( y^{[k]}(x) \) is \( 2^k \) in the variables \( x \). Then, by the chain rule, one can write the gradient operator of the reduced-degree integral

\[
\nabla \tilde{H}(x, y^{[1]}, \ldots, y^{[n_y]}) = \left( \frac{\partial}{\partial x} + \left( \frac{\partial y^{[1]}(x)}{\partial x} \right)^T \frac{\partial}{\partial y^{[1]}(x)} + \ldots + \left( \frac{\partial y^{[n_y]}(x)}{\partial x} \right)^T \frac{\partial}{\partial y^{[n_y]}(x)} \right) \tilde{H}(x, y^{[1]}, \ldots, y^{[n_y]})
\]

(10)

where \( \frac{\partial y^{[k]}(x)}{\partial x} \) is the Jacobian derivative matrix of \( y^{[k]}(x) \) with respect to \( x \). The reduced-degree ODE for \( x \) with respect to \( \tilde{H}(x, y^{[1]}, \ldots, y^{[n_y]}) \) is therefore

\[
\dot{x} = S(x) \nabla \tilde{H}(x, y^{[1]}, \ldots, y^{[n_y]}) := f(x, y^{[1]}, \ldots, y^{[n_y]})
\]

which satisfies the consistency condition \( f(x, y^{[1]}(x), \ldots, y^{[n_y]}(x)) = f(x) \). Although it is not needed for our method, the corresponding ODEs for the \( y^{[k]} \) variables that make up the extended system are

\[
y^{[k]} = \frac{\partial y^{[k]}(x)}{\partial x} f(x, y^{[1]}, \ldots, y^{[n_y]}) \quad \text{for} \quad k = 1, \ldots, n_y.
\]

This, together with \( \dot{x} \) form an extended system that possesses the induced quadric integrals \( H_{i,j} = y^{[k]}_{i,j} - y^{[k-1]}_{i} y^{[k-1]}_{j} \). As each \( H_{i,j} \) as well as the reduced degree Hamiltonian \( \tilde{H} \) are all quadratic then the midpoint rule \( x' \) preserves these integrals. Therefore we can immediately solve for \( (y^{[k]})' \) in terms of \( x' \). Inserting this solution yields the reduced-degree midpoint rule for polynomial integrals

\[
\frac{x' - x}{h} = f \left( \frac{x' + x}{2} - \frac{y^{[1]}(x') + y^{[1]}(x)}{2}, \ldots, \frac{y^{[n_y]}(x') + y^{[n_y]}(x)}{2} \right),
\]

(11)

the solution to which satisfies \( H(x') = H(x) \).

### 2.2.1 Example: the octic oscillator

Consider the oscillator with Hamiltonian

\[
H(x_1, x_2) = \frac{1}{2} x_1^2 + \frac{1}{8} x_2^8 \in \mathbb{R}[x_1, x_2]
\]

that corresponds to the ODE

\[
\begin{align*}
\dot{x}_1 &= -x_2^7, \\
\dot{x}_2 &= x_1.
\end{align*}
\]

(12)

Now introduce the variables \( y^{[1]}_{2,2} = x_2 \) and \( y^{[2]}_{2,2,2,2} = \left( y^{[1]}_{2,2} \right)^2 \) to define the following reduced-degree Hamiltonian

\[
\tilde{H}(x_1, x_2, y^{[1]}_{2,2}, y^{[2]}_{2,2,2,2}) = \frac{1}{2} x_1^2 + \frac{1}{8} \left( y^{[2]}_{2,2,2,2} \right)^2 \in \mathbb{R}[x_1, x_2, y^{[1]}_{2,2}, y^{[2]}_{2,2,2,2}]
\]
The reduced-degree vector field of \( \tilde{H}(x_1, x_2, y_2^{[1]}, y_2^{[2]}, y_{2,2,2,2}) \) is therefore
\[
\begin{align*}
\dot{x}_1 &= -x_2 y_2^{[1]} y_2^{[2]}, \\
\dot{x}_2 &= x_1.
\end{align*}
\]
(13)

The corresponding extended system possesses the induced quadric integrals \( H_{2,2} = y_2^{[1]} - x_2^2 \) and \( H_{2,2,2,2} = y_{2,2,2,2}^2 - \left( y_2^{[1]} \right)^2 \). Therefore the midpoint method satisfies \( y_2^{[1]} = x_2^2 \) and \( y_{2,2,2,2}^2 = \left( y_2^{[1]} \right)^2 \). Applying the reduced-degree midpoint rule (11) to (13) yields
\[
\begin{align*}
\frac{x_1' - x_1}{2h} &= -\left( \frac{x_2' + x_2}{2} \right) \left( \frac{x_2' + x_2^2}{2} \right) \left( \frac{x_2'^2 + x_2^4}{2} \right), \\
\frac{x_2' - x_2}{2h} &= \frac{x_1' + x_1}{2},
\end{align*}
\]
the solution to which satisfies \( H(x_1', x_2') = H(x_1, x_2) \). We remark that this method is also identical to the averaged vector field method.

2.3 Preservation of multiple integrals

The idea behind the reduced-degree midpoint rule is simply to introduce auxiliary quadratic variables to write the system as an equivalent extended system that possesses only quadric integrals, then apply the midpoint rule and use the quadratic-integral-preserving property to exactly project the map back onto the original phase space. This can be applied directly to ODEs with multiple first integrals, therefore extending the reduced-degree midpoint method (11) to preserve multiple polynomial integrals is straightforward. Given an ODE with \( m = n \) first integrals \( H_i(x) \in \mathbb{R}_d[x] \) for \( i = 1, ..., m \), then it is always possible to write the ODE in the following multi-skew-gradient form [3][22]
\[
\dot{x} = S(\nabla H_1(x), ..., \nabla H_m(x))
\]
where \( S \) is some skew-symmetric \( m + 1 \) tensor that may depend on \( x \). That is, \( S_{i_0, ..., i_k, ..., i_m} = -S_{i_0, ..., i_k, ..., i_m}, \) for any \( j, k = 0, ..., m \). To find a suitable \( S \), one can use a symbolic algebra software package such as Maple or Matlab, or use a more heuristic approach outlined in [3][22], for example.

To create an integral preserving method, we start by writing down the \( m \) reduced-degree integrals \( \tilde{H}_i(x, y^{[1]}, ..., y^{[n_m]}) \in \mathbb{R}_2[x, y^{[1]}, ..., y^{[n_m]}] \). The reduced-degree ODE is therefore
\[
\dot{x} = S(\nabla \tilde{H}_1, ..., \nabla \tilde{H}_m) := f(x, y^{[1]}, ..., y^{[n_m]})
\]
where the vectors \( \nabla \tilde{H}_i \) are functions of \( (x, y^{[1]}, ..., y^{[n_m]}) \) and are calculated by equation (10). Then the reduced-degree midpoint rule from equation (11) applied to \( f(x, y^{[1]}, ..., y^{[n_m]}) \) preserves all integrals \( H_i \) for \( i = 1, ..., m \). Examples are given in section 3.

2.4 Higher-order methods

After defining the reduced-degree vector field and the extended ODE system (e.g., equation (3)) one can apply any symplectic Runge-Kutta method and project the solution onto the original \( n \)
dimensional phase space to yield an integral-preserving method. However, if we implement higher-
order symplectic Runge-Kutta methods, it becomes difficult to avoid calculation of the stage values
for the $y^{[k]}$ equations and therefore results in a method that requires the numerical solution of a
non-linear system in a much higher dimensional phase space than the original ODE, which is slow.
As we have seen in section 2.1 the midpoint rule is a special because we can avoid solving the
$y^{[k]}$ equations, and their subsequent stage values, by substituting in the solutions $y'_{i,j} = x'_i x'_j$
that solve the superfluous equations. There are other Runge-Kutta methods that share this property,
namely the diagonally-implicit symplectic Runge-Kutta (DISRK) methods. Such methods have
Butcher table of the form

$$
\begin{array}{c|cccc}
 c_1 & b_1/2 & 0 & 0 & \ldots & 0 \\
c_2 & \vdots & \ddots & \ddots & \ddots & \vdots \\
c_{s-1} & b_1 & b_2 & \ldots & b_{s-1} & b_s/2 \\
c_s & \vdots & \ddots & \ddots & \ddots & \vdots \\
\end{array}
$$

(14)

that is, with $a_{ii} = b_i/2$, $a_{ij} = b_j$ for $i < j$ and $a_{ij} = 0$ otherwise. These methods are by
construction symplectic. Moreover, due to theorem 4.4 in [1, p. 192] a Runge-Kutta method $\Phi_h$
with coefficients given by (14) is equivalent to compositions of the midpoint rule, which we denote
by $\Phi^M_h$, with sub-steps $b_i h$. That is,

$$
\Phi_h = \Phi^M_{b_s h} \circ \cdots \circ \Phi^M_{b_2 h} \circ \Phi^M_{b_1 h}.
$$

(15)

This means that one can construct high-order reduced-degree Runge-Kutta methods without the
need to solve the stage values for the $y^{[k]}$ equations by taking compositions of the reduced-degree
midpoint rule.

In addition to the above DISRK methods, due to the fact that the midpoint rule is symmetric, one
can use composition [29] to create methods of higher order, in a similar way to equation (15) [1].
This is demonstrated in [3].

2.5 Connection with averaged vector field method.

Another popular energy-preserving method for Hamiltonian systems that is of particular interest
to the present paper is the averaged vector field (AVF) method, given by

$$
\frac{x' - x}{h} = \int_0^1 f((1 - \xi)x + \xi x') d\xi,
$$

(16)

which was introduced in [8]. In [30] it is shown that the AVF method coincides with the Runge-
Kutta method whose Butcher coefficients correspond with the nodes and weights of a quadrature
rule applied to the integral in (16). It turns out that the AVF method is a special case of the
reduced-degree midpoint method when applied to Hamiltonian ODEs with quartic Hamiltonian
due to the following.
Proposition 1. Consider a planar Hamiltonian ODE of the form \( H(\mathbf{x}) = 0 \) with the general quartic Hamiltonian

\[
H(\mathbf{x}) = \alpha_1 x_1 + \alpha_2 x_2 + \alpha_3 x_1^2 + \alpha_4 x_1 x_2 + \alpha_5 x_2^2 + \alpha_6 x_1^3 + \alpha_7 x_1^2 x_2 + \alpha_8 x_1 x_2^2 + \alpha_9 x_2^3 + \alpha_{10} x_1^4 + \alpha_{11} x_1^3 x_2 + \alpha_{12} x_1^2 x_2^2 + \alpha_{13} x_1 x_2^3 + \alpha_{14} x_2^4
\]

where \( \alpha_i \in \mathbb{R} \) are arbitrary and consider the following reduced-degree Hamiltonian

\[
\tilde{H}(\mathbf{x}, \mathbf{y}) = \alpha_1 x_1 + \alpha_2 x_2 + \alpha_3 x_1^2 + \alpha_4 x_1 x_2 + \alpha_5 x_2^2 + \alpha_6 x_1 y_{1,1} + \alpha_7 (\beta_1 y_{1,1} x_2 + (1 - \beta_1) y_{1,2} x_1) + \alpha_8 (\beta_2 y_{2,2} x_1 + (1 - \beta_2) y_{1,2} x_2) + \alpha_9 x_2 y_{2,2}
\]

\[
+ \alpha_{10} y_{1,1}^2 + \alpha_{11} y_{1,1} y_{1,2} + \alpha_{12} (\beta_3 y_{1,2}^2 + (1 - \beta_3) y_{1,1} y_{2,2}) + \alpha_{13} y_{2,2} y_{1,2} + \alpha_{14} y_{2,2}^2
\]

where \( \beta_2, \beta_3 \in \mathbb{R} \) are free parameters. Then the reduced-degree midpoint rule corresponding to \( \tilde{H}(\mathbf{x}, \mathbf{y}) \) coincides with the AVF method when \( \beta_1 = \beta_2 = 1/3 \) and \( \beta_3 = 2/3 \).

Proof. This can be seen by direct computation. \( \square \)

We have also observed similar results for Hamiltonians up to degree eight, although this has been omitted due to space constraints. The fact that the reduced-degree midpoint rule yields the AVF method implies that it is also a Runge-Kutta method for such choices of parameters. Of course, the reduced-degree midpoint rule is not a Runge-Kutta method in general, e.g., when applied to ODEs with non-constant Poisson structure. It remains an interesting endeavor to further elucidate the connection between the reduced-degree midpoint method for canonical Hamiltonian ODEs, the AVF and their underlying Runge-Kutta methods.

3 Numerical examples

This section comprises of three numerical examples. The first is a planar Hamiltonian ODE, where we compare the reduced-degree midpoint method against some other geometric integrators for Hamiltonian systems. The second example is of a Nambu system and is designed to illustrate the full capabilities of our method. Here, we have designed a vector field with bounded orbits in three dimensions that possesses two integrals of degree four and eight. We implement higher-order reduced-degree methods of up to degree eight using DISRK methods and symmetric composition and compare them to the standard methods of equal order. The final example is of the famous Toda lattice system from quantum mechanics. Here, we show that we can numerically integrate the system while preserving all integrals.

3.1 A planar quartic-Hamiltonian ODE

In this example we will consider a planar Hamiltonian ODE given by

\[
\begin{align*}
\dot{x}_1 &= -2 x_1^2 x_2 - 4 x_2^3 \\
\dot{x}_2 &= 2 x_1 x_2^2 + x_1
\end{align*}
\]

\[
:= f(\mathbf{x})
\]

where the Hamiltonian function is \( H(\mathbf{x}) = \frac{1}{2} x_1^2 + x_2^4 + x_1^2 x_2 \). Then defining the reduced-degree Hamiltonian \( \tilde{H}(\mathbf{x}, \mathbf{y}) = x_1^2/2 + y_2^2 + \alpha_1 y_{1,1} y_{2,2} + (1 - \alpha) y_{2,2}^2 \) for \( \alpha \in \mathbb{R} \) a free parameter, we can derive the corresponding reduced-degree ODE system by equation (3)

\[
\begin{align*}
\dot{x}_1 &= -2 ((1 - \alpha) x_1 y_{1,1} + \alpha x_2 y_{1,1}) - 4 x_2 y_{2,2} \\
\dot{x}_2 &= 2 (\alpha x_1 y_{2,2} + (1 - \alpha) x_2 y_{1,1}) + x_1
\end{align*}
\]

\[
:= f(\mathbf{x}, \mathbf{y})
\]
We now apply the reduced-degree midpoint rule, defined by equation (6), and set \( \alpha = 0 \) which yields

\[
\begin{align*}
\frac{x_1' - x_1}{h} &= -2 \left( \frac{x_1' + x_1}{2} \right) \left( \frac{x_1 x_2' + x_1 x_2}{2} \right) - 4 \left( \frac{x_2' + x_2}{2} \right) \left( \frac{x_2 x_2' + x_2 x_2}{2} \right), \\
\frac{x_2' - x_2}{h} &= 2 \left( \frac{x_2' + x_2}{2} \right) \left( \frac{x_1 x_2' + x_1 x_2}{2} \right) + \left( \frac{x_1' + x_1}{2} \right).
\end{align*}
\]

Numerical simulations using the reduced-degree midpoint method (RD-MP2) are presented in

![Numerical orbits of the quartic Hamiltonian ODE (17) (first row) and the corresponding errors to the Hamiltonian (second row). The columns correspond to the midpoint rule (first column), Simpson’s rule (second column) and the reduced-degree midpoint method (third column). The black and red dots are the initial conditions, red meaning that the numerical solution becomes unstable during the \( n = 10^4 \) time steps. The time step is \( h = 1/10 \).](image)

Figure 2: Numerical orbits of the quartic Hamiltonian ODE (17) (first row) and the corresponding errors to the Hamiltonian (second row). The columns correspond to the midpoint rule (first column), Simpson’s rule (second column) and the reduced-degree midpoint method (third column). The black and red dots are the initial conditions, red meaning that the numerical solution becomes unstable during the \( n = 10^4 \) time steps. The time step is \( h = 1/10 \).

As the ODE is Hamiltonian, there exist a number of methods with good structure-preserving properties for comparison. We will use the standard midpoint method (MP2) as well as AVF method. The midpoint method is symplectic and therefore has bounded Hamiltonian error. The AVF method preserves the Hamiltonian and is also a Runge-Kutta method, known as Simpson’s method [10], and corresponds to evaluating the integral in (16) with Gaussian quadrature of order 4. Furthermore, we remark that the RD-MP2 method with \( \alpha = 1/3 \) also yields the AVF method. All methods solve the resulting implicit equations using fixed point iterations with an absolute tolerance of \( 1.11 \times 10^{-15} \). Using a time step of \( h = 1/10 \), a total of 13 numerical orbits are plotted from the initial conditions \( \mathbf{x}_0^{(i)} = (2 + 2i/3, 0)^T \), for \( i = 0, \ldots, 12 \) denoted by black dots. Red dots denote those initial conditions where the solution becomes unstable. We see that the midpoint method loses stability for the initial conditions corresponding to \( i = 8, \ldots, 12 \), the AVF
method loses stability for \(i = 10, \ldots, 12\) while the reduced-degree midpoint method retains stability for all initial conditions. We note that all three methods are unstable when \(i = 13\). Figure 2 also shows the Hamiltonian error as a function of simulation time. We see that the reduced-degree midpoint method and the Simpson method preserves the Hamiltonian up to machine precision for their stable orbits, whereas the standard midpoint rule does not. Lastly, we note that different choices of \(\alpha\) affect the stability and accuracy of the method.

### 3.2 A Nambu system with two integrals

In this next example, we have designed an ODE with bounded orbits possessing two integrals, one of degree four and one of degree eight. The ODE is given by

\[
\begin{align*}
\dot{x}_1 &= 8x_2^3x_3 (x_1^4 + x_3^2) (x_2^2 - 1) - 2x_2 (2x_3x_4^2 + x_1) (x_1^2 + 2x_2^2 + x_3^2 - 1) \\
\dot{x}_2 &= 2x_1 (x_2^2 - 1) (2x_3x_2 + x_1) - 2x_3 (x_2^2 - 1) (4x_1^2x_3^2 + x_3) \\
\dot{x}_3 &= 2x_2 (4x_1^3x_2^2 + x_3) (x_2^2 - 1) - 8x_1x_3 (x_1^4 + x_3^2) (x_2^2 - 1)
\end{align*}
\]

(18)

and the integrals are

\[
\begin{align*}
H_1(x) &= x_1^4x_2^4 + x_1x_3 + x_2^4x_3^2 \\
H_2(x) &= (x_2^2 - 1) (x_1^2 + x_2^2 + x_3^2)
\end{align*}
\]

Now consider the following reduced-degree integrals

\[
\tilde{H}_1(x, y^{[1]}, y^{[2]}) = y_1^{[2]} y_2^{[2]} y_3^{[1]}, y_1^{[1]} + y_2^{[2]} y_3^{[1]} \\
\tilde{H}_2(x, y^{[1]}, y^{[2]}) = (y_2^{[1]} - 1) (y_1^{[1]} + y_2^{[1]} + y_3^{[1]})
\]

where \(y^{[1]} = (y_1^{[1]}, y_2^{[1]}, y_3^{[1]})^T\) and \(y^{[2]} = (y_1^{[2]}, y_2^{[2]}, y_3^{[2]})^T\). This yields the following reduced-degree vector field of \(\mathbf{f}(x)\)

\[
\dot{x} = \mathbf{f}(x, y^{[1]}, y^{[2]})
\]

\[
= \begin{pmatrix}
8x_2x_3y_2^{[1]}y_3^{[3]} + y_2^{[1]}y_1^{[1]}y_3^{[1]}(y_2^{[2]} - 1) - 2x_2(x_1 + 2x_3y_2^{[2]})(y_1^{[1]} + 2y_2^{[1]} + y_3^{[1]} - 1) \\
2x_1(x_2 + 2x_3y_2^{[2]})(y_2^{[1]} - 1) - 2x_3(x_3 + 4x_1y_1^{[1]}y_2^{[2]})(y_2^{[2]} - 1) \\
2x_2(x_3 + 4x_1y_1^{[1]}y_2^{[2]})(y_1^{[1]} + 2y_2^{[1]} + y_3^{[3]} - 1) - 8x_1x_2y_2^{[1]}y_3^{[3]}y_1^{[1]}y_3^{[1]}(y_2^{[2]} - 1)
\end{pmatrix}
\]

In addition to the midpoint method, we also consider the following higher-order methods. The first is a three-stage fourth-order DISRK method (DISRK4)

\[
b_1 = (\sqrt{2} + \sqrt{2} + 2)/3, \quad b_2 = 1 - 2b_1, \quad b_3 = b_1,
\]

the second is an eleven-stage sixth-order DISRK method (DISRK6) \[31\]

\[
b_1 = 0.6152247129651358, \quad b_2 = -0.9769283017304923, \quad b_3 = 0.775622228585488, \\
b_4 = 1.1870793818191547, \quad b_5 = -1.1292359636503542, \quad b_6 = 0.05647589547601459, \\
b_7 = b_5, \quad b_8 = b_4, \quad b_9 = b_3, \quad b_{10} = b_2, \quad b_{11} = b_1,
\]
and the third is a 15-stage eighth-order composition method (C8) [32]

\[\begin{align*}
    b_1 &= 0.7416703643506129, & b_2 &= -0.4091008258000315, & b_3 &= 0.1907547102962383, \\
    b_4 &= -0.5738624711160822, & b_5 &= 0.299064183036559, & b_6 &= 0.3346249182452981, \\
    b_7 &= 0.315293023967665, & b_8 &= -0.7968879393529163, \\
    b_9 &= b_7, & b_{10} &= b_6, & b_{11} &= b_5, & b_{12} &= b_4, & b_{13} &= b_3, & b_{14} &= b_2, & b_{15} &= b_1.
\end{align*}\]

A total of eight numerical methods are implemented. The first four are the conventional MP2, DISRK4, DISRK6 and C8 methods applied to the original ODE (18). The latter four methods are the reduced-degree versions of these methods, denoted by RD-MP2, RD-DISRK4, RD-DISRK6 and RD-C8. The methods are implemented as compositions of the RD-MP2 method (11) or the standard MP2 method by equation (15). Using the initial condition \(x_0 = (1/2, 1/2, 1/2)^T\) and over the time interval \([0, 1]\), the convergence of the six methods are tested and the results are displayed in figure 3a. Here, we observe all the expected orders. From the same initial conditions, the numerical solutions are calculated over the time interval \([0, 100]\) with a stepsize of \(h = 1/20\). The numerical solutions are plotted in figure 4. Here we see that the RD methods remain on the intersection of the two isosurfaces \(H_1(x) = H_1(x_0)\) and \(H_2(x) = H_2(x_0)\), whereas the conventional methods drift off. The integral errors \(H_i(x_k) - H_i(x_0)\) are presented in figure 3b. We see that the RD methods preserve the integrals to within machine precision, while the conventional methods do not. Furthermore, the MP2 and DISRK4 methods lose stability early on in the simulation.

![Figure 3: The convergence of the eight methods after one second of simulation time for varying h (a) and the errors \(H_1(x_k) - H_1(x_0)\) (solid lines) and \(H_2(x_k) - H_2(x_0)\) (dashed lines) during 100 seconds of simulation time for \(h = 1/20\) (b). The black dashed lines in figure (a) are orders two, four, six and eight.](image)

### 3.3 Toda Lattice \((N = 3)\)

One of the most famous integrable systems in physics is the Toda lattice. Integrable disretisations of this system have been studied in, for example [33]. Consider a Toda lattice of \(N = 3\) particles...
Figure 4: Numerical phase lines of the ODE using the numerical methods starting from $x_0 = (1/2, 1/2, 1/2)^T$ with $h = 1/20$. The composition methods (C8 and RD-C8) yield visually similar figures to that figures (d), (e) and (f).

with periodic boundary conditions in the variables $x = (a_1, a_2, a_3, b_1, b_2, b_3)^T$. This is given by

$$
\dot{a}_1 = a_1 (b_2 - b_1), \\
\dot{a}_2 = a_2 (b_3 - b_2), \\
\dot{a}_3 = a_3 (b_1 - b_3), \\
\dot{b}_1 = a_1 - a_3, \\
\dot{b}_2 = a_2 - a_1, \\
\dot{b}_3 = a_3 - a_2.
$$

This ODE possesses the following integrals

$$
H_1 = b_1 + b_2 + b_3, \\
H_2 = a_1 a_2 a_3, \\
H_3 = \frac{1}{3} (b_3^3 + b_1^3 + b_2^3) + a_1 b_1 + a_2 b_2 + a_3 b_3 + a_1 b_2 + a_2 b_3 + a_3 b_1, \\
H_4 = \frac{1}{2} (b_1^2 + b_2^2 + b_3^2) + a_1 + a_2 + a_3.
$$

two of which are cubic. Quadratic reduced-degree Hamiltonians can be written by introducing the variables $y_{1,2} = a_1 a_2$, $y_{4,4} = b_1^2$, $y_{5,5} = b_2^2$ and $y_{6,6} = b_3^2$ and the skew-symmetric 5-tensor components $S_{i_0,i_1,i_2,i_3,i_4}$ are found using a a symbolic software program such as Maple, see also [3][22] for details on the construction of this tensor. Using a time step of $h = 1/10$ starting from initial conditions
\( x_0 = (1, 2, 3, 4, 5, 6)/6 \) we implement the reduced-degree midpoint method. Figure 5 shows the errors of the integrals \( \Delta H_i = |H_i(x_k) - H_i(x_0)| \) for \( i = 1, \ldots, 4 \). We see that all four integrals are preserved to machine precision. We remark that the choice of \( S_{i_0,i_1,i_2,i_3,i_4} \) is not unique and it is important to choose one that is sufficiently regular to avoid issues with the numerical solution of the implicit equations.

![Figure 5: The errors of the integrals of the \( N = 3 \) Toda lattice.](image)

### 4 Discussion and conclusion

In this paper we have introduced the reduced-degree midpoint method, which is a novel numerical integrator for solving ODEs while preserving all polynomial first integrals. We have shown that using DISRK methods, we can develop higher-order integral-preserving reduced-degree methods. The reduced-degree methods are tested on a number of numerical examples including the Toda lattice. In all examples we see conservation of all polynomial integrals up to machine precision.

The reduced-degree midpoint method is a Runge-Kutta method, but applied to a higher dimensional ODE, whose solution solves the original ODE under study. Due to this, the method inherits the same properties as the midpoint rule such as time-symmetry, affine equivariance and a B-series, however what is not clear is how these properties on the extended phase space relate to the original ODE. This would be an interesting topic for a future study. For the considered polynomial Hamiltonian systems, we have observed that the reduced-degree midpoint rule yields the AVF method as a special case, which implies that the reduced-degree midpoint rule is a Runge-Kutta method on the original phase space for these ODEs and parameter choice. However, this is clearly not the case for ODEs with non-constant Poisson structure. An interesting question is therefore when does the reduced-degree midpoint rule yield a Runge-Kutta method on the original phase space. In contrast to the AVF method, the presented method can preserve multiple integrals and is applicable to ODEs other than Hamiltonian. The connection between the reduced degree midpoint method and the AVF method awaits further investigation.

The idea behind the reduced-degree midpoint rule can be applied to ODEs with invariants other than polynomial first integrals. In [34] it is shown that all Runge-Kutta methods preserve all affine second integrals (also known as Darboux polynomials [35]) and rational affine first integrals. Therefore, by introducing reduced-degree affine second integrals as well as reduced degree rational affine first integrals, one should be able to create a method that preserves all rational integrals of a given ODE. We hope to present this method in a future study [36].
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