Geometric integration methods that unconditionally contract volume

V. Grimm *, G.R.W. Quispel

[a] *Department of Mathematics, and Centre for Mathematics and Statistics of Complex Systems*
La Trobe University
Bundoora, Melbourne 3086, Australia

Abstract

We consider ordinary differential equations (ODEs) that contract volume in phase space. It is very hard to construct geometric integrators which inherit this property of the exact flow for all volume contracting ODEs, and so far no integrators have been known with this property. In this work we present some integrators of this type.

Key words: Geometric integration; Volume-preserving system; Splitting method; Projection method

1 Introduction

In recent years, there has been much interest in geometric integration, the numerical integration of differential equations while preserving one or more (geometric) properties exactly (i.e. up to round-off error). Recent surveys on geometric integration are given in Budd & Piggott [1], Hairer, Lubich & Wanner [5], Leimkuhler & Reich [6], Quispel & McLachlan (eds.) [10], Sanz-Serna & Calvo [12]. Most publications on geometric integration concern dynamical systems that can be considered 'conservative'. However, there has also been some work on 'dissipative' systems, eg on integrators that preserve Lyapunov functions, contract phase-space volume, or decrease some norm of the solution

* Corresponding author's current address: Mathematisches Institut, Heinrich-Heine Universität Düsseldorf, Universitätsstraße 1, D-40225 Düsseldorf, Germany

Email addresses: grimm@am.uni-duesseldorf.de (V. Grimm), R.Quispel@latrobe.edu.au (G.R.W. Quispel).

(cf. Grimm & Quispel [4], McLachlan & Quispel [8], Stuart and Humphries [16]). In the current paper we derive novel methods that unconditionally contract volume in phase space for appropriate systems.

Consider the ODE

$$\dot{y} = f(y), \qquad y(0) = y_0, \qquad y \in \mathbb{R}^n \tag{1}$$

with solution $y(t)$ and Jacobian $A(t) = \partial y(t)/\partial y(0)$ which evolves according to

$$\dot{A} = FA, \qquad A(0) = I,$$

where $F(t) = F(y(t)) = \partial f(y(t))/\partial y$ is the derivative of the vector field f evaluated at the exact solution. We have

$$\frac{d}{dt} \det A \;=\; \det A \operatorname{tr} F, \qquad \det A\,(0) = 1, \tag{2}$$

so that phase space volume contracts, is preserved, or expands when $\operatorname{tr} F < 0$, $\operatorname{tr} F = 0$, or $\operatorname{tr} F > 0$ for all y, respectively. $\operatorname{tr} F = \operatorname{div} f$ is the trace or divergence of the vector field f. System (1) is said to be (weakly) contractive, if $\operatorname{div} f \leq 0$. From (2), one can find that in this case

$$0 < \det A \leq 1.$$

As mentioned in [8], all consistent numerical integrators by application on strongly contractive systems (i.e. $\operatorname{tr} F < b < 0$) will be contractive for small enough time step h. The authors of [8] considered weakly contractive systems and gave the following definition, where $B = \partial \Psi_h/\partial y$ is the Jacobian of the numerical one-step method Ψ_h.

Definition 1 *The ODE (1) is (weakly) contractive if* $\operatorname{tr} F \leq 0$ *for all* y. *An integrator is (weakly) contractive if for any matrix norm* $\|\cdot\|$ *and all* $L > 0$ *there is a time step* $h^* > 0$ *such that* $|\det B| \leq 1$ *for all* $0 \leq h \leq h^*$, *for all* y *and for all* f *such that* $\|F\| < L$ *and* $\operatorname{tr} F \leq 0$.

In [8], it is mentioned that it is prohibitively difficult to require contractivity of an integrator for all contractive vector fields and for *all* $h > 0$. We will show that integrators of this type exist. But even more, we ask for integrators whose determinant stays between 0 and 1, as does the determinant of the exact solution. The definition above only asks for the absolute value of the determinant to be in the correct range. Precisely, we examine the question whether unconditionally contractive integrators, according to the following definition, exist.

Definition 2 *An integrator is unconditionally (weakly) contractive if* $0 < \det B \leq 1$ *for all* $0 < h$, *for all* y *and for all* f *such that* $\operatorname{tr} F \leq 0$.

The definition is given in the same sense as the definition of A-stability. That is, there might be another condition restricting h, for example computability of the approximation, but the important thing is, that the requirement of being contractive does not restrict the step size h.

In this paper we present two different unconditionally contractive integration methods. We present an efficient but low-order composition method in Section 2, and we present a (less efficient but) higher-order projection method in Section 4. For each of these methods we present numerical experiments in Section 3, resp. 5. Volume-preserving methods are known for being hard to find and a volume-contracting method should be a volume-preserving method if applied to the special case of divergence 0. These methods are (new) volume-preserving methods in this special case. The application of these methods involves some preparation which might include the use of symbolic software to differentiate and integrate polynomials. After some more numerical experiments in Section 5, we give a conclusion in Section 6.

2 The splitting method

The basic idea of the following splitting method is to split the equation in two parts, a volume-preserving vector field and a one-dimensional vector field that contracts volume. The volume-preserving vector field $f^{[1]}$ reads:

$$\begin{aligned}
\dot{y}_1 &= f_1(y_1, \cdots, y_n) - \textstyle\int_0^{y_1} \operatorname{div} f(x_1, y_2, \cdots, y_n)\, dx_1 \\
\dot{y}_2 &= f_2(y_1, \cdots, y_n) \\
&\vdots \\
\dot{y}_n &= f_n(y_1, \cdots, y_n).
\end{aligned}$$

The one-dimensional vector field $f^{[2]}$ that contracts volume is given by

$$\begin{aligned}
\dot{y}_1 &= \textstyle\int_0^{y_1} \operatorname{div} f(x_1, y_2, \cdots, y_n)\, dx_1 \\
\dot{y}_2 &= 0 \\
&\vdots \\
\dot{y}_n &= 0.
\end{aligned}$$

The volume-preserving vector field can be computed by one of the known volume-preserving integrators (cf. [3,8,9,11,14,15]). For example, if one chooses the implicit midpoint rule $\Psi_h^{[1]}$ as a volume-preserving integrator for the vector field $f^{[1]}$ and the backward Euler method $\Psi_h^{[2]}$ for the contracting vector field

$f^{[2]}$, it is easy to see that the methods $\Psi_h^{[1]} \circ \Psi_h^{[2]}$ and $\Psi_h^{[2]} \circ \Psi_h^{[1]}$ are unconditionally contractive and of order 1. If the solution enters a domain D where the differential equation is volume preserving, that is div $f(y) = 0$ for $y \in D$, then the backward Euler method reduces to the identity and the composed methods are volume preserving. Proposition 3 shows that unconditionally contractive methods of order 2 can be constructed with this splitting.

Proposition 3 *If one chooses a volume-preserving integrator $\Psi_h^{[1]}$ of order 2 or higher to approximate the volume-preserving vector field $f^{[1]}$ and an integrator $\Psi_h^{[2]}$ of order 2 or higher that is unconditionally contracting for one-dimensional vector fields (such as $f^{[2]}$), then the compositions*

$$\Psi_{h/2}^{[1]} \circ \Psi_h^{[2]} \circ \Psi_{h/2}^{[1]} \qquad \textit{and} \qquad \Psi_{h/2}^{[2]} \circ \Psi_h^{[1]} \circ \Psi_{h/2}^{[2]}$$

are unconditionally contractive integrators of order 2 for the vector field f. If the method $\Psi_h^{[2]}$ solves differential equations with zero right-hand side exactly, then the compositions reduce to volume-preserving integrators wherever the vector field is volume-preserving.

Proof Since method $\Psi_h^{[1]}$ approximates the flow of the ODE with vector field $f^{[1]}$ with order 2 or higher and $\Psi_h^{[2]}$ approximates the flow of the ODE with vector field $f^{[2]}$ with order 2 or higher, the compositions in the proposition approximate the composition of the exact flows at least with order 2. But the compositions of the exact flows are known to approximate the flow of the differential equation to order two (cf. [7]). The reduction to volume-preserving integrators is obvious. □

In order to use Proposition 3, it remains to show that there are unconditionally contractive integrators of second order for one-dimensional systems. This is done in Lemma 1.

Lemma 1 *The implicit Runge-Kutta method*

$$y_1 = y_0 + hf(y_1 - \tfrac{h}{2} f(y_1))$$

is unconditionally contractive for one-dimensional systems, and has order 2. The method integrates systems with zero right-hand side exactly.

Proof The order can be seen easily by using the tableau or by computing the Taylor series of the numerical method. The derivative $\frac{\partial y_1}{\partial y_0}$ satisfies the equation

$$\frac{\partial y_1}{\partial y_0} = 1 + h \frac{\partial f}{\partial y}(y_1 - \tfrac{h}{2} f(y_1)) \left(\frac{\partial y_1}{\partial y_0} - \frac{h}{2} \frac{\partial f}{\partial y}(y_1) \frac{\partial y_1}{\partial y_0} \right),$$

or

$$\left(1 - h \frac{\partial f}{\partial y}(y_1 - \tfrac{h}{2} f(y_1)) + \tfrac{h^2}{2} \frac{\partial f}{\partial y}(y_1 - \tfrac{h}{2} f(y_1)) \frac{\partial f}{\partial y}(y_1) \right) \frac{\partial y_1}{\partial y_0} = 1,$$

or

$$\frac{\partial y_1}{\partial y_0} = \frac{1}{1 - h\frac{\partial f}{\partial y}(y_1 - \frac{h}{2}f(y_1)) + \frac{h^2}{2}\frac{\partial f}{\partial y}(y_1 - \frac{h}{2}f(y_1))\frac{\partial f}{\partial y}(y_1)}.$$

Hence

$$0 < \frac{\partial y_1}{\partial y_0} \leq 1.$$

The last inequality follows since

$$-\frac{\partial f}{\partial y}(x) \geq 0 \qquad \text{and} \qquad \frac{\partial f}{\partial y}(x)\frac{\partial f}{\partial y}(z) \geq 0$$

holds for all x and z and volume-contracting one-dimensional vector fields (that is $\partial f(x)/\partial y \leq 0$). □

3 A numerical experiment

The ODE

$$\begin{aligned} \dot{x} &= -10(x + \cos x) - y \\ \dot{y} &= x, \end{aligned}$$

is used as a simple test equation. The splitting reads

$$\begin{aligned} \dot{x} &= -y & \qquad \dot{x} &= -10(x + \cos x) \\ \dot{y} &= x & \qquad \dot{y} &= 0. \end{aligned}$$

The implicit midpoint method is used for the volume-preserving vector field and the Runge-Kutta method in Lemma 1 for the volume-contracting vector field. The second splitting in Proposition 3 is chosen.

Note that the implicit midpoint rule Ψ_h alone is volume-preserving but not unconditionally volume contractive. This can easily be seen for the test equation $\dot{y} = -y := f(y)$ with $\operatorname{div} f = -1 < 0$ but

$$\det \frac{\partial \Psi_h}{\partial y} = \frac{1 - \frac{h}{2}}{1 + \frac{h}{2}} < 0$$

for $h > 2$.

The splitting method is now compared to the (weakly) contracting midpoint method. Figure 1 shows the determinant of the derivative of the numerical flow as a function of time for the implicit midpoint method and the splitting method. Again one can see that the implicit midpoint method is not unconditionally volume-contractive whereas the determinants of the splitting method stay nicely between 0 and 1. The starting values are $(x_0, y_0) = (0, 1000)$.

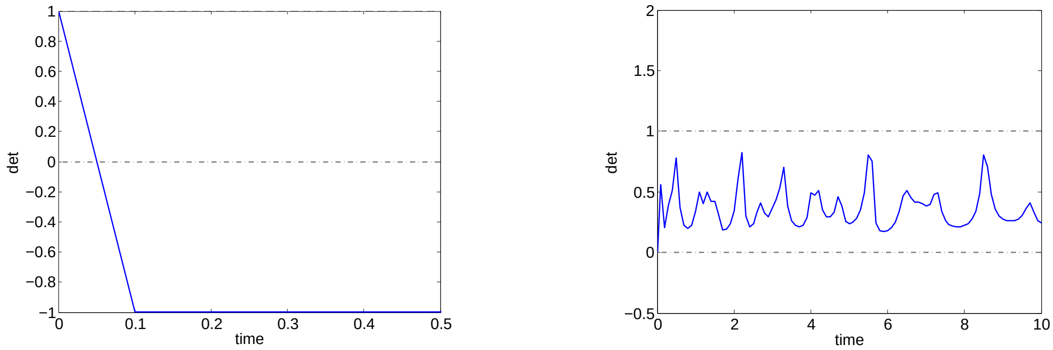

Fig. 1. Determinants of the implicit midpoint (left) and the splitting method (right) with $h = 0.1$

The order of the methods is shown in Figure 2, using starting values $(x_0, y_0) = (2\pi, 2\pi)$ and an interval of length 1.

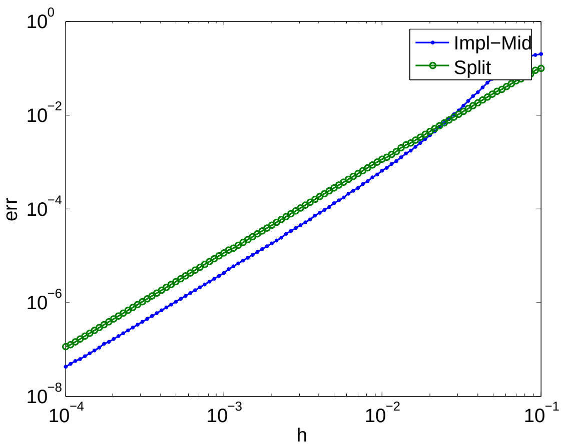

Fig. 2. Error versus step size for the implicit midpoint and the splitting method

4 Projection method

The construction of higher-order unconditionally contractive methods is based on the following idea. A base numerical method is designated by $y = \Phi_h(y'')$. Another map, called the projector, by $y' = C_h(y)$. Here, primes are used to designate different variables and not derivatives. The projector is chosen with respect to the numerical method in such a way that the projected method $y' = \Psi_h(y'') := C_h \circ \Phi_h(y'')$ is unconditionally volume-contracting and of the same order as method Φ_h.

The projector C_h is determined by two functions F and G.

$$\begin{aligned} y_1' &= y_1 \\ \vdots &= \vdots \\ y_{n-1}' &= y_{n-1} \\ F(y_1, \cdots, y_{n-1}, y_n') &= G(y_1, \cdots, y_{n-1}, y_n) \end{aligned} \tag{3}$$

Theorem 4 shows that a projector can be found for all Runge-Kutta methods that have an explicit adjoint with nonnegative coefficients. The functions F and G have to be determined only once before starting the numerical integration. If the vector field f in (1) is polynomial, so are the functions F and G.

As usually, the Runge-Kutta method $y = \Phi_h(y'')$, computed as

$$\begin{aligned} g_i &= y'' + h \textstyle\sum_{j=1}^s a_{ij} f(g_j), \qquad i = 1 \ldots s, \\ y &= y'' + h \textstyle\sum_{i=1}^s b_i f(g_i), \end{aligned}$$

is denoted by its tableaux

$$\begin{array}{c|c} c & A \\ \hline & b \end{array} \quad = \quad \begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array}$$

The adjoint method Φ_h^* is then given by the tableaux

$$\begin{array}{c|c} c^* & A^* \\ \hline & b^* \end{array} \quad = \quad \begin{array}{c|c} \mathbb{1} - Pc & \mathbb{1}bP - PAP \\ \hline & bP \end{array},$$

where $\mathbb{1} = [1, \cdots, 1]^T$ and P is the permutation matrix that flips the order of a vector.

Three examples of Runge-Kutta methods to that Theorem 4 applies are given here together with their adjoint. The tableau of the method Φ_h, used in Lemma 1, reads

$$
\begin{array}{c}
\Phi_h \\[1em]
\begin{array}{c|cc}
\frac{1}{2} & 1 & -\frac{1}{2} \\
1 & 1 & 0 \\
\hline
 & 1 & 0
\end{array}
\end{array}
\qquad\qquad
\begin{array}{c}
\Phi_h^* \\[1em]
\begin{array}{c|cc}
0 & 0 & 0 \\
\frac{1}{2} & \frac{1}{2} & 0 \\
\hline
 & 0 & 1
\end{array}
\end{array}
\tag{4}
$$

Φ_h^* designates the adjoint method. The method $\widehat{\Phi}_h$, which has a well-known Heun method as adjoint $\widehat{\Phi}_h^*$, is unconditionally contractive for one-dimensional systems and of order 3.

$$
\begin{array}{c}
\widehat{\Phi}_h \\[1em]
\begin{array}{c|ccc}
\frac{1}{3} & \frac{3}{4} & -\frac{2}{3} & \frac{1}{4} \\
\frac{2}{3} & \frac{3}{4} & 0 & -\frac{1}{12} \\
1 & \frac{3}{4} & 0 & \frac{1}{4} \\
\hline
 & \frac{3}{4} & 0 & \frac{1}{4}
\end{array}
\end{array}
\qquad\qquad
\begin{array}{c}
\widehat{\Phi}_h^* \\[1em]
\begin{array}{c|ccc}
0 & 0 & & \\
\frac{1}{3} & \frac{1}{3} & 0 & \\
\frac{2}{3} & 0 & \frac{2}{3} & 0 \\
\hline
 & \frac{1}{4} & 0 & \frac{3}{4}
\end{array}
\end{array}
\tag{5}
$$

The method $\tilde{\Phi}_h$, which has "the" Runge-Kutta method as adjoint $\tilde{\Phi}_h^*$, is unconditionally contractive for one-dimensional systems and of order 4.

$$
\begin{array}{c}
\tilde{\Phi}_h \\[1em]
\begin{array}{c|cccc}
0 & \frac{1}{6} & \frac{1}{3} & -\frac{2}{3} & \frac{1}{6} \\
\frac{1}{2} & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & -\frac{1}{3} \\
\frac{1}{2} & \frac{1}{6} & -\frac{1}{6} & \frac{1}{3} & \frac{1}{6} \\
1 & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6} \\
\hline
 & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6}
\end{array}
\end{array}
\qquad\qquad
\begin{array}{c}
\tilde{\Phi}_h^* \\[1em]
\begin{array}{c|cccc}
0 & 0 & & & \\
\frac{1}{2} & \frac{1}{2} & 0 & & \\
\frac{1}{2} & 0 & \frac{1}{2} & 0 & \\
1 & 0 & 0 & 1 & 0 \\
\hline
 & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6}
\end{array}
\end{array}
\tag{6}
$$

Theorem 4 *For a Runge-Kutta method Φ_h, whose adjoint is an explicit method (i.e. $a_{ij}^* = 0$ for $i \leq j$) and has nonnegative coefficients (i.e. $a_{ij}^* \geq 0, b_i^* \geq 0$), we can find functions F and G in (3) such that the method $\Psi_h = C_h \circ \Phi_h$ is unconditionally volume-contracting and of the same order as method Φ_h. If the vector field f is polynomial, then F and G are polynomials (that can be easily determined using symbolic software). The method reduces to a volume-preserving integrator wherever the vector field is volume preserving.*

Proof First, the original system (1) is augmented in the following way,

$$\begin{aligned} \dot{y} &= f(y), & y(0) &= y'' \\ \dot{d} &= \operatorname{div} f(y)\, d, & d(0) &= 1 \end{aligned}$$

$d(h, y_0)$, the component corresponding to d in the exact solution, is the same as the determinant of the Jacobian of the exact solution of system (1), that is

$$d(h, y_0) = \left| \frac{\partial y(h)}{\partial y(0)} \right|.$$

Here and in the remainder of the proof, we denote the determinant of a matrix A as $|A|$. For our systems, we have $0 \le d(h, y_0) \le 1$ for all y_0 and $h \ge 0$. Since the methods under consideration are of order p for arbitrary ODEs, it holds that

$$\left\| d_1(h, y_0) - \left| \frac{\partial y(h)}{\partial y_0} \right| \right\| = O(h^{p+1}),$$

where d_1 designates the numerical solution component corresponding to d.

Now let

$$F(y_1, \cdots, y_n') = \int_0^{y_n'} \frac{1}{d_1(h, \Phi_h^{-1}(y_1, \cdots, \bar{y}_n))}\, d\bar{y}_n$$

and

$$G(y_1, \cdots, y_n) = \int_0^{y_n} \left| \frac{\partial \Phi_h}{\partial y_n''} \left(\Phi_h^{-1}(y_1, \cdots, \bar{y}_n \right) \right|^{-1} d\bar{y}_n.$$

We are looking at the solution of the equation

$$\int_0^{y_n'} \frac{1}{d_1(h, \Phi_h^{-1}(y_1, \cdots, \bar{y}_n))}\, d\bar{y}_n = \int_0^{y_n} \left| \frac{\partial \Phi_h}{\partial y_n''} \left(\Phi_h^{-1}(y_1, \cdots, \bar{y}_n \right) \right|^{-1} d\bar{y}_n.$$

First of all, one has that $\Phi_h^{-1} = \Phi_{-h}^*$, that is, the inverse is the adjoint method applied with negative step size h. Furthermore, there is a close relationship between the internal stages $\tilde{g} = [\tilde{g}_1, \cdots, \tilde{g}_s]^T$ of $y'' = \Phi_h^{-1}(y) = \Phi_{-h}^*(y)$ and the internal stages $g = [g_1, \cdots, g_s]^T$ of $y = \Phi_h(y'')$, namely $g = P\tilde{g}$. This will now be used to examine $d_1(h, y'') = d_1(h, \Phi_h^{-1}(y_1, \cdots, y_n))$. This approximation of the determinant can be written as

$$d_1(h, y'') = 1 + bZ(I - AZ)^{-1}\mathbb{1} =: K(Z),$$

where

$$Z = \operatorname{diag}(h \operatorname{div} f(g_1), \cdots, h\, f \operatorname{div} f(g_s)).$$

We now have

$$\frac{1}{d_1(h, \Phi_h^{-1}(y))} = K(Z)^{-1} = K(-P\tilde{Z}P)^{-1} = 1 + b^*\tilde{Z}(I - A^*\tilde{Z})^{-1}\mathbb{1} =: K^*(\tilde{Z}),$$

with

$$\tilde{Z} = \operatorname{diag}\left(-h \operatorname{div} f(\tilde{g}_1), \cdots, -h \operatorname{div} f(\tilde{g}_s)\right).$$

Since A^*, b^* are nonnegative and belong to an explicit method, it follows that $K^*(\tilde{Z}) \geq 1$ and that $K^*(\tilde{Z})$ is a polynomial in y, whenever the vector field f is. Furthermore,

$$0 < d_1(h, y'') = d_1(h, \Phi_h^{-1}(y)) \leq 1.$$

For the second integrand, we have

$$\begin{aligned}\left(\frac{\partial \Phi_h}{\partial y_n''}(\Phi_h^{-1}(y_1, \cdots, y_n))\right)^{-1} &= \frac{\partial \Phi_h^{-1}}{\partial y_n''}(y_1, \cdots, y_n) \\ &= \frac{\partial \Phi_{-h}^*}{\partial y_n''}(y_1, \cdots, y_n).\end{aligned}$$

The last term can easily be seen to be a polynomial in $(y_1, \cdots, y_n)$, if the vector field f is. (Differentiation of the explicit recursion to compute Φ_{-h}^* gives the explicit recursion for the Jacobian).

Furthermore, it is clear that

$$d_1(h, \Phi_h^{-1}(y_1, \cdots, y_n)) = \left|\frac{\partial y(h, \Phi_h^{-1}(y_1, \cdots, y_n))}{\partial y_0}\right| + O(h^{p+1}),$$

as well as

$$\left|\frac{\partial \Phi_h}{\partial y''}(\Phi_h^{-1}(y_1, \cdots, y_n))\right| = \left|\frac{\partial y(h, \Phi_h^{-1}(y_1, \cdots, y_n))}{\partial y_0}\right| + O(h^{p+1}).$$

Replacing these in our equation above shows that

$$\|y' - y\| = \|y_n' - y_n\| = O(h^{p+1}),$$

that is, the projection does not decrease the order of the underlying method.

Finally, the determinant of Ψ_h satisfies

$$\left|\frac{\partial \Psi_h}{\partial y''}\right| = \left|\frac{\partial C_h}{\partial y}\right| \cdot \left|\frac{\partial \Phi_h}{\partial y''}\right|,$$

but

$$\left|\frac{\partial C_h}{\partial y}\right| = \frac{\partial y_n'}{\partial y_n} = d_1(h, \Phi_h^{-1}(y_1, \cdots, y_{n-1}, y_n')) \cdot \left|\frac{\partial \Phi_h}{\partial y''}(\underbrace{\Phi_h^{-1}(y_1, \cdots, y_{n-1}, y_n)}_{=y''})\right|^{-1}.$$

Hence

$$\begin{aligned}\left|\frac{\partial \Psi_h}{\partial y''}(y'')\right| &= d_1(h, \Phi_h^{-1}(y_1, \cdots, y_{n-1}, y_n')) \cdot \left|\frac{\partial \Phi_h}{\partial y''}(y'')\right|^{-1} \left|\frac{\partial \Phi_h}{\partial y''}(y'')\right| \\ &= d_1(h, \Phi_h^{-1}(y_1, \cdots, y_{n-1}, y_n')).\end{aligned}$$

That is

$$0 \leq \left| \frac{\partial \Psi_h}{\partial y''} \right| \leq 1,$$

and furthermore,

$$\begin{aligned} d_1(h, \Phi_h^{-1}(y_1, \cdots, y_{n-1}, y_n')) &= d_1(h, \Phi_h^{-1}(y_1, \cdots, y_{n-1}, y_n)) + O(h^{p+1}) \\ &= \left| \frac{\partial y(h, y'')}{\partial y(0)} \right| + O(h^{p+1}), \end{aligned}$$

that is, the determinant is an $O(h^{p+1})$-approximation to the correct determinant.

In a region D where the vector field is volume preserving, that is $\operatorname{div} f(y) = 0$ for $y \in D$, we have $d_1(h, y'') = 1$ since Runge-Kutta methods solve ODEs with zero right-hand side exactly. Hence

$$\left| \frac{\partial \Psi_h}{\partial y''} \right| = 1$$

and the method is volume preserving. □

Remark: The function $K(Z)$ that appears in the proof is related to the AN-stability function of the Runge-Kutta method Φ_h (cf. [2,13]). This can be seen if $\operatorname{div} f(y)$ is regarded as a time-dependent but not solution-dependent function. The function $K^*(Z)$ is then related to the AN-stability function of the adjoint method Φ_h^*.

5 A numerical experiment with the projection method

The ODE

$$\begin{aligned} \dot{x} &= (-\tfrac{8}{5}x^5 + \tfrac{8}{3}x^3 - 2x) - y \\ \dot{y} &= x, \end{aligned}$$

is used as a simple test equation, with starting values $(x_0, y_0) = (2, 0)$. Figure 3 shows the determinant of the derivative of the numerical flow of the implicit midpoint method on the left hand side and of the new unconditionally contractive method based on $\hat{\Phi}_h$ on the right hand side. Figure 4 displays the order of the methods. A last experiment checks the rate of contraction. In Figure 5, the continuous line shows the exact value for $\det \partial y(t)/\partial y(0)$, computed with a standard integrator set to high accuracy. At $t_n = hn$, $\prod_{i=1}^{n} \det \partial\Phi_h(y_n)/\partial y_n$ is an approximation for this value and shows how accurately the infinitesimal contraction of the exact solution is represented by the numerical method. The midpoint method on the left hand side of Figure 5 does not correctly represent the overall contraction. The new projected method, displayed on the right hand side, is close to the exact contraction rate.

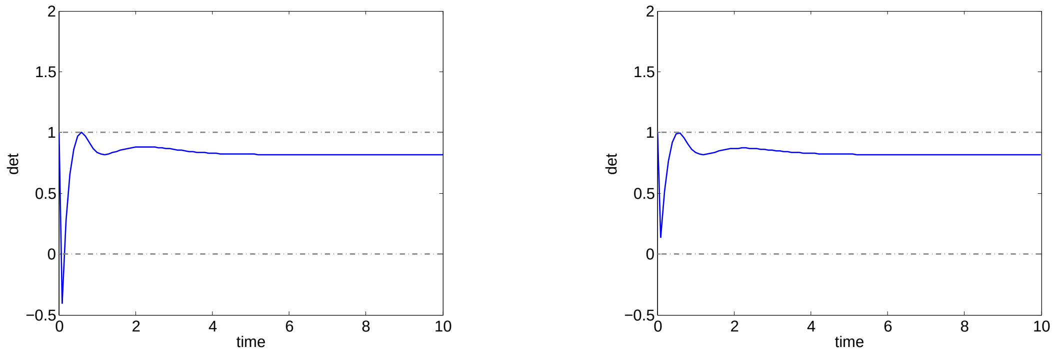

Fig. 3. Determinants of the implicit midpoint (left) and the projected method of order 3 (right) with $h = 0.1$

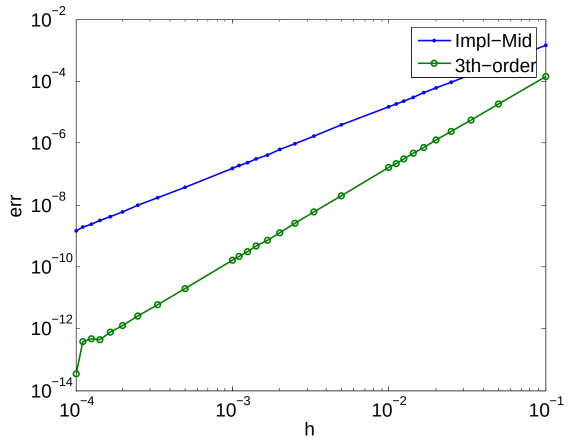

Fig. 4. Error versus step size for the implicit midpoint and the projected method of order 3

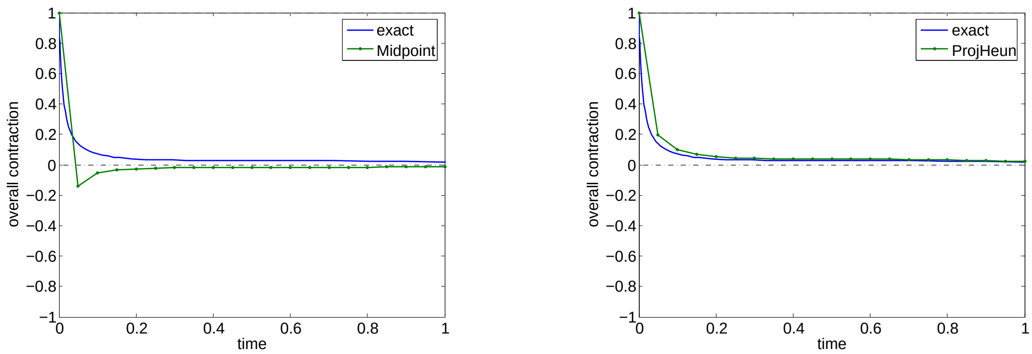

Fig. 5. Contraction of phase space volume for the implicit midpoint (left) and the projected method of order 3 (right) with $h = 0.1$

6 Conclusion

We presented some methods that are unconditionally volume-contractive. As far as we know, these are the first methods that have this property even when the contraction can be arbitrarily small. The new integrators are a unification in the sense that they reduce to volume-preserving methods if they are applied to a volume-preserving vector field. As volume-preserving integrators the projection methods are also new.

Acknowledgement: We are grateful to the Australian Research Council for financially supporting this research.

References

[1] C.J. Budd and M.D. Piggott, *Geometric integration and its applications*, Proceedings of ECMWF workshop on "Developments in numerical methods for very high resolution global models", pp. 93-118, 2000.

[2] K. Burrage and J.C. Butcher, *Stability criteria for implicit Runge-Kutta methods*, SIAM J. Numer. Anal., Vol. 16, pp. 46-57, 1979.

[3] K. Feng and Z. Shang, *Volume-preserving algorithms for source-free dynamical systems*, Numer. Math., Vol. 71, pp. 451-463, 1995.

[4] V. Grimm and G.R.W. Quispel, *Geometric Integration Methods that Preserve Lyapunov Functions*, BIT, Vol. 45, pp. 709-723, 2005.

[5] E. Hairer, Ch. Lubich and G. Wanner, *Geometric Numerical Integration*, 2nd edition, Springer-Verlag, 2006.

[6] B. Leimkuhler and S. Reich, *Simulating Hamiltonian Dynamics*, Cambridge University Press, 2004.

[7] R.I. McLachlan and G.R.W. Quispel, *Splitting methods*, Acta Numerica, Vol. 11, pp. 341-434, 2002.

[8] R.I. McLachlan and G.R.W. Quispel, *Numerical integrators that contract volume*, Appl. Num. Math., Vol. 34, pp. 253-260, 2000.

[9] M.-Z. Qin and W.-J. Zhu, *Volume-preserving schemes and numerical experiments*, Comput. Math. Appl., Vol. 26, pp. 33-42, 1993.

[10] G.R.W. Quispel and R.I. McLachlan (eds.), *Geometric Numerical Integration of Differential Equations*, J. Phys. A: Math. Gen., Vol. 39, 2006.

[11] G.R.W. Quispel, *Volume-preserving integrators*, Phys. Lett. A, Vol. 206, pp. 26-30, 1995.

[12] J.M. Sanz-Serna and M.P. Calvo, *Numerical Hamiltonian Problems*, Chapman & Hall, 1994.

[13] R. Scherer, *A necessary condition for B-stability*, BIT, Vol. 19, pp. 111-115, 1979.

[14] Z. Shang, *Generating functions for volume-preserving mappings and Hamilton-Jacobi equations for source-free dynamical systems*, Sci. China Ser. A 37, pp. 1172-1188, 1994.

[15] Z. Shang, *Construction of volume-preserving difference schemes for source-free systems via generating functions*, J. Comput. Math., Vol. 12, pp. 256-272, 1994.

[16] A.M. Stuart and A.R. Humphries, *Dynamical Systems and Numerical Analysis*, Cambridge Univ. Press, 1996.