Volume Preserving Methods

Brynjulf Owren

July 26, 2015

Volume preserving flows. A theorem by Liouville states that Hamiltonian systems preserve volume in phase space. A Hamiltonian vector field is divergence free which is easily seen for the canonical form since

$$\mathrm{div}(J^{-1}\nabla H) = \sum_{i=1}^{d}\left(\frac{\partial}{\partial q_i}\dot{q}_i + \frac{\partial}{\partial p_i}\dot{p}_i\right) = \sum_{i=1}^{d}\left(\frac{\partial}{\partial q_i}\frac{\partial H}{\partial p_i} + \frac{\partial}{\partial p_i}\left(-\frac{\partial H}{\partial q_i}\right)\right) = 0.$$

In fact, it is true that all divergence free systems preserve volume in phase space

Theorem 1. *Let $\dot{y} = f(y)$ be a system of ODEs on $\mathbb{R}^d$. Let $D \subset \mathbb{R}^d$ be open and bounded, let φ_t be the flow of f and set*

$$D(t) = \varphi_t(D), \quad \textit{and} \quad v(t) = \mathrm{vol}(D(t)) = \int_{D(t)} \mathrm{d}V$$

If $\mathrm{div} f = 0$ then $v(t) = v(0)$ for all $t > 0$.

Proof. Expanding the solution $y(t)$ with initial value $y(0) = y$ to the first order yields $y(t) = \varphi_t(y) = y + tf(y) + \mathcal{O}(t^2)$. The formula for changing variables in multiple integrals gives

$$v(t) = \int_{D(0)} \det\left(\frac{\partial \varphi_t}{\partial y}\right) \mathrm{d}V$$

Differentiating the expansion to the first order of $y(t)$ with respect to y we find

$$\frac{\partial \varphi_t}{\partial y} = I + \frac{\partial f}{\partial y} t + \mathcal{O}(t^2) \text{ as } t \to 0.$$

For any matrix A we have

$$\det(I + tA) = 1 + t\sum_i a_{ii} + \mathcal{O}(t^2) = 1 + t\,\mathrm{tr}(A) + \mathcal{O}(t^2)$$

Consequently

$$\det\frac{\partial \varphi_t}{\partial y} = \det\left(I + t\frac{\partial f}{\partial y} + \mathcal{O}(t^2)\right) = 1 + t\,\mathrm{tr}\left(\frac{\partial f}{\partial y}\right) + \mathcal{O}(t^2)$$

Since $\mathrm{tr}(\partial f/\partial y) = \mathrm{div} f$, we get

$$v(t) = \int_{D(0)} \left(1 + t\,\mathrm{div} f + \mathcal{O}(t^2)\right) \mathrm{d}V$$

so

$$\left.\frac{\mathrm{d}v}{\mathrm{d}t}\right|_{t=0} = \int_{D(0)} \mathrm{div} f \, \mathrm{d}V$$

The argument can be repeated for any $t_0 > 0$ and we simply get

$$\left.\frac{\mathrm{d}v}{\mathrm{d}t}\right|_{t=t_0} = \int_{D(t_0)} \mathrm{div} f \, \mathrm{d}V$$

so for divergence free f we conclude that $\frac{\mathrm{d}v}{\mathrm{d}t} = 0$ and $v(t) \equiv$ constant. □

Example 1 A popular volume preserving problem is the ABC-flow

$$\begin{aligned} \dot{x} &= A \sin z + C \cos y \\ \dot{y} &= B \sin x + A \cos z \\ \dot{z} &= C \sin y + B \cos x \end{aligned} \tag{1}$$

Since the ith component of the vector field is independent of the ith variable, we have $\mathrm{div} f = 0$. □

Here are some known facts about volume preserving integrators which we do not prove

1. Symplectic integrators are volume preserving for Hamiltonian vector fields, but not for all divergence free vector fields
2. No "standard method" can be volume preserving for all divergence free vector fields in $\mathbb{R}^n$.
3. All known volume preserving numerical methods do some kind of preprocessing to the vector field, typically they exploit some information that can be extracted from each particular problem.

Example 2 A particularly simple type of divergence free problems is

$$\dot{y} = Ay, \quad A \in \mathbb{R}^{d\times d} \text{ and } \mathrm{tr}(A) = 0. \tag{2}$$

Runge-Kutta methods for this problem, and possibly also other types of methods will typically use some analytic function $R(z)$, and set $y_1 = \Phi_h(y_0) = R(hA)y_0$. You already know that for the Euler method $R(z) = 1 + z$ and for the implicit midpoint rule, $R(z) = \frac{1+z/2}{1-z/2}$. Let D_0 be an open bounded set in $\mathbb{R}^d$, and let $D_1 = \Phi_h(D_0)$. As in the proof of Liouville's theorem, we get

$$\mathrm{vol}(D_1) = \int_{D_0} \det \frac{\partial \Phi_h}{\partial y_0} \, \mathrm{d}V = \int_{D_0} \det R(hA) \, \mathrm{d}V$$

so this means we must require $\det R(hA) = 1$ for the method to be volume preserving.

It turns out that the set of $d \times d$-matrices of unit determinant is a Lie group called $SL(d)$, whereas its Lie algebra is precisely the linear space of divergence free $d \times d$-matrices, called $\mathfrak{sl}(d)$. Finding a volume-preserving integrator for the problem (2) amounts to searching for a function $R(z)$ which maps $\mathfrak{sl}(d)$ to $SL(d)$. A well-known result by Feng and Shang shows that there are no such differentiable maps, satisfying $R(0) = R'(0) = 1$ [1, Lemma IV.3.2], the original source is [2]. $\square$

Volume preserving numerical methods. We have already referred to the 1995-paper of Feng and Shang [2]. In this paper, a pioneering construction of volume preserving integrators is also devised. We shall largely follow the presentation in [1].

Theorem 2. *(Feng & Shang 1995). Every divergence free vector field $f : \mathbb{R}^d \to \mathbb{R}^d$ can be written as a sum of $d-1$ vector fields*

$$f = f_{1,2} + f_{2,3} + \cdots + f_{d-1,d}$$

each $f_{k,k+1}$ being Hamiltonian in (y_k, y_{k+1}), that is, one can find

$$H_{k,k+1} : \mathbb{R}^d \to \mathbb{R}$$

such that

$$f_{k,k+1} = (0, \ldots, 0, -\frac{\partial H_{k,k+1}}{\partial y_{k+1}}, 0, \ldots, 0)^T$$

the non-zero entries being no k and $k+1$.

For a general constructive proof of the theorem, we refer to [1, 2], but let us do the construction for the ABC-flow presented earlier. We start by comparing the first component of (1) with the first vector field $f_{1,2}$ which has $-\partial H_{12}/\partial y$ as its first component.

$$-\frac{\partial H_{1,2}}{\partial y} = A \sin z + C \cos y \quad \Leftarrow \quad H_{1,2} = -Ay \sin z - C \sin y$$

Note that we could also have added an "integration constant" $\zeta(x, z)$, but it turns out not to be necessary. Instead we consider the second component of f in the theorm which will have contributions both from $f_{1,2}$ and $f_{2,3}$. Comparing with the second component of (1), we get

$$\frac{\partial H_{1,2}}{\partial x} - \frac{\partial H_{2,3}}{\partial z} = B \sin x + A \cos z$$

We substitute the found expression for $H_{1,2}$ and integrate with respect to z, but this time we must include a constant of integration in order to tackle the last component

$$\frac{\partial H_{2,3}}{\partial z} = -A \sin x - A \cos z \quad \Leftrightarrow \quad H_{2,3} = -Bz \sin x - A \sin z + \zeta(x, y)$$

Finally, we need to consider the third component

$$\frac{\partial H_{2,3}}{\partial y} = \frac{\partial \zeta}{\partial y}(x,y) = C\sin y + B\cos z \quad \Leftarrow \quad \zeta(x,y) = -C\cos y + B\,y\cos x$$

So we conclude that

$$H_{2,3} = -Bz\sin x - A\sin z - C\cos y + By\cos x$$

Splitting methods and groups of diffeomorphisms. We did not yet explain the reason why Theorem 2 is useful. The reason can be found in a class of methods called splitting methods which is somewhat similar to composition methods. As mentioned before, certain important classes of problems, such as Hamiltonian problems or divergence free problems, have flows which belong to a group under composition. These groups are subgroups of the space of all diffeomorphisms. It turns out that the set of all vector fields whose flows belong to such a subgroup is a linear space. Let us denote such a linear space of vector fields by $\mathfrak{g}$ and the corresponding group by G. Keep in mind the example that G consist of symplectic maps, and $\mathfrak{g}$ of Hamiltonian vector fields. If $f \in \mathfrak{g}$ and there are two other vector fields also in $\mathfrak{g}$ such that

$$\dot{y} = f(y) = f_1(y) + f_2(y),$$

then an approximation to the flow $\exp(hf) := \varphi_h$ for small h would be

$$\exp(hf) = \exp(hf_1) \circ \exp(hf_2) + \mathcal{O}(h^2)$$

One can make more elaborate compositions such as

$$\exp(\frac{h}{2}f_1) \circ \exp(hf_2) \circ \exp(\frac{h}{2}f_1)$$

known under the name *Strang splitting*, it has (formally) second order convergence. One can boot-strap to even higher order by using a trick due to Yoshida [3]. It is of course also possible to use splitting methods when the vector field has been split into a sum of more than two terms. The important observation is, however, that if the flow of each term can be computed exactly, then it will belong to the group G which is closed under composition, so the composed flow will again belong to G. But one can also replace the exact flow e.g. $\exp(hf_k)$ of the kth term by some numerical method of the right type, i.e. such that $\Phi_{h,f_k} \in G$. Finally, we may now apply the splitting idea to the Feng-Shang splitting of a divergence free vector field into a sum of $d-1$ simple vector fields as described in Theorem 2. In two dimensions, volume preservation is the same as symplecticity, so if we either compute the flows of $f_{k,k+1}$ exactly, or replace them by a symplectic scheme (letting all components of y except y_k, y_{k+1} be constant), and compose them all in the manner of a splitting method. We can work out the details for the ABC-flow. Let us write down each of the problems corresponding to $f_{1,2}$ and $f_{2,3}$

$f_{1,2}$	$f_{2,3}$
$\dot{x} = A\sin z + C\cos y$	$\dot{x} = 0$
$\dot{y} = 0$	$\dot{y} = B\sin x + A\cos z$
$\dot{z} = 0$	$\dot{z} = C\sin y + B\cos x$

The first flow can be computed exactly, we see that

$$\exp(hf_{1,2})\mathbf{y}_0 = (x_0 + h(A \sin z_0 + C \cos y_0), y_0, z_0)^T$$

The second can be approximated by some symplectic scheme, because volume preservation is the same as symplecticity in two dimensions. We also notice that the system is separable in the variables y, z so e.g. the symplectic Euler method can be implemented in an explicit manner

$$\begin{aligned}
x_{n+1} &= x_n \\
y_{n+1} &= y_n + h(B \sin x_n + A \cos z_n) \\
z_{n+1} &= z_n + h(C \sin y_{n+1} + B \cos x_n)
\end{aligned}$$

References

[1] Ernst Hairer, Christian Lubich, and Gerhard Wanner. *Geometric numerical integration*, volume 31 of *Springer Series in Computational Mathematics*. Springer, Heidelberg, 2010. Structure-preserving algorithms for ordinary differential equations, Reprint of the second (2006) edition.

[2] Feng Kang and Zai Jiu Shang. Volume-preserving algorithms for source-free dynamical systems. *Numer. Math.*, 71(4):451–463, 1995.

[3] H. Yoshida. Construction of higher order symplectic integrators. *Physics Letters A*, 150:262–268, 1990.