Numerical volume preservation of a divergence free fluid under symmetry
Mattheij, R.M.M.; Laevsky, K.

Published: 01/01/2001

Document Version
Publisher's PDF, also known as Version of Record (includes final page, issue and volume numbers)

Please check the document version of this publication:
• A submitted manuscript is the author's version of the article upon submission and before peer-review. There can be important differences between the submitted version and the official published version of record. People interested in the research are advised to contact the author for the final version of the publication, or visit the DOI to the publisher's website.
• The final author version and the galley proof are versions of the publication after peer review.
• The final published version features the final layout of the paper including the volume, issue and page numbers.
Link to publication

Citation for published version (APA):

General rights
Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.
• Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
• You may not further distribute the material or use it for any profit-making activity or commercial gain
• You may freely distribute the URL identifying the publication in the public portal

Take down policy
If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Download date: 07. Dec. 2018

R.M.M. Matttheij, K. Laevsky
Department of Mathematics and Computer Science,
Eindhoven University of Technology,
PO Box 513, 5600 MB The Netherlands

Abstract

This paper studies conservative formulations for the evolution of flows in 3-D which satisfy a symmetry condition. It is shown how the Hamiltonian form leads to a proper form of the evolution equation. This is illustrated by a number of examples. It is also shown how this results in conservation of e.g. mass when using simplectic integrators. A special section is devoted to computing displacements by the implicit midpoint rule when the velocities are not available in explicit form but e.g. found from a numerical method like FEM.

1 Introduction

In a large variety of fluid mechanical problems one encounters volumes or areas that are conserved during their evolution. Typically this occurs for incompressible flows, where the conservation of mass and momentum results in the equations of motion [7]. Since we obtain a velocity field from these equations we are faced with the problem of finding the evolution, i.e., the displacement and deformation, of a body from this velocity field in a conservative way from the ordinary differential equation (ODE)

\[ \frac{dx}{dt} = v(x(t)), \]  

(1.1)

where \( x \) is a point in the volume and \( v \) the velocity. Although (1.1) looks deceivingly simple, it does not lend itself for easy numerical computation (see [5], [6], [8], [14]). For one thing, the variable \( x \) is an element in a continuum (in contrast to the usual finite number of trajectories). Hence it is not easy, at least not trivial computationally, to use an implicit time discretisation. To fix thoughts, if we have a body with a moving boundary, it is this boundary that we would like to compute. We would first need to make at least a guess, needed to use this implicit method as a corrector (see e.g. [7]). But this boundary is a continuum, not just a finite number of trajectories.

Quite another problem, and the main topic of this paper, is the concern how to preserve the mass numerically. From numerical ODE theory we know that there exist a number of methods which preserve the volume of a flow (see [2], [3], [6], [13]) more or less satisfactorily. In particular there are so called simplectic integrators, which are closely linked to Hamiltonian forms (cf. [1], [13]); we shall restrict ourselves to the implicit midpoint rule here, which is good enough to demonstrate our case. It is important to remark that the theory of simplectic methods deals with finite dimensional systems of even order. It is possible to generalize this to two-dimensional volumes (i.e. rather areas). For a three dimensional problem the underlying Hamiltonian theory is essentially impossible, as it requires an even order space (see [1]). In this paper we shall describe a way
to deal with bodies in a physically three dimensional space, only requiring some form of symme-
try. We shall employ the fact that such a problem can typically be reduced to a two dimensional
problem, which in turn may be solved by a simplectic method as mentioned above.

This paper is built up as follows. In Section 2 we consider the relationship between conservation
and the stream function as a Hamiltonian. Then in Section 3 we consider problems defined in
cylindrical coordinates. Using axissymmetry we show how to formulate a Hamiltonian form. This
is worked out in some numerical examples. Also for spherical coordinates employing symmetry
is obvious. For the latter we also deal with axial symmetry in Section 4. Again we show how we
can employ this to obtain conservation of volume. This is illustrated by a Stokes flow around a
sphere. The last case we discuss is where we have spherical symmetry, see Section 5. Although
this case deals with patches on a sphere rather than volumes in 3-D it employs similar ideas as in
the two other cases. The final part of the paper, Section 6, is devoted to a method that describes
how to use an implicit method, like the midpoint rule, if the velocity field is not explicitly given.
It is based on employing the fact that the velocity field is usually autonomous (i.e. not time
dependent). Numerical examples illustrate that this method de facto preserves volumes, even if
\( v \) is found from a numerical method, say FEM. We may conclude that simplectic methods will
improve the numerical accuracy of the computed “conserved quantities” beyond the order of the
discretisation error.

2 Hamiltonian Systems

For our discussion we shall consider incompressible fluids. The continuity equation for a fluid
body with density \( \rho \) and velocity \( v \) is then given by \( \nabla \cdot \rho v = 0 \). For homogeneous density this
simplifies to

\[
\nabla \cdot v = 0. \tag{2.1}
\]

If \( V(t) \) denotes a certain volume at time \( t \) with surface \( S(t) \), then we know that

\[
\int_{V(t)} \nabla \cdot v \, dv = \int_{S(t)} v \cdot n \, dS = 0. \tag{2.2}
\]

Clearly, the net outflow is zero, i.e. \( V(t) \) is constant. Let \( x(t) = (x(t), y(t))^T \in V(t) \) be a point in
Cartesian coordinates with a velocity

\[
v := (u_x(x, y), u_y(x, y))^T. \tag{2.3}
\]

Then (2.1) implies

\[
\frac{\partial}{\partial x} u_x + \frac{\partial}{\partial y} u_y = 0. \tag{2.4}
\]

This can be associated to a stream function, \( \psi(x, y) \) say (see [4]), with

\[
\begin{align*}
  u_x &= -\frac{\partial \psi}{\partial y}, \\
  u_y &= \frac{\partial \psi}{\partial x},
\end{align*} \tag{2.5}
\]

Since \( u_x = dx/dt \) and \( u_y = dy/dt \) we have the system of ordinary differential equations
Although we may not (wish to) know $\psi$, we do note that the system underlying (1.1) is in fact (2.6), a Hamiltonian form. So a divergence-free two dimensional velocity field implies a simplectic form for a point in that field. There is a host of literature on Hamiltonian systems, see [1], [3], [13]. We only use the fact that they preserve a flow volume. The latter property has to do with the two dimensional volume $V(t)$ in which $(x, y)^T$ runs. It is well known that one can use simplectic numerical integrators which are also volume preserving. In this paper we will restrict ourselves to the implicit midpoint rule which reads for (2.6) (using (2.5))

$$
\begin{align*}
\frac{dx}{dt} &= -\frac{\partial \psi}{\partial y}, \\
\frac{dy}{dt} &= \frac{\partial \psi}{\partial x}.
\end{align*}
$$

(2.6)

Here $\Delta t$ is the time step and $k$ is the time level. This method is of the second order in $\Delta t$ (see [6], [13]). For a linear system (2.7) will give a conservation of flow volume, for nonlinear systems this is not necessarily so; still it is often gives near conservation, see [13].

From the very form of (2.6) it is clear that we cannot hope to have a Hamiltonian form for a three dimensional vector. Yet, for the problems which have some kind of symmetry we can reduce the order often by 1 so that a de facto two dimensional problem remains. This is the subject of the next three sections.

3 Hamiltonians for 3-D Axisymmetric Cases: Cylindrical Coordinates

The most common types of symmetry in fluid problems are cylindrical and spherical symmetry. We shall consider the first one in this section, the second one in the next two.

We use cylindrical coordinates $r$, $z$, $\varphi$ as radial, axial, and angular variables respectively. Consider the continuity equation in cylindrical coordinates

$$
\nabla \cdot \mathbf{v} = \frac{1}{r} \frac{\partial}{\partial r}(ru_r) + \frac{\partial}{\partial z}u_z + \frac{1}{r} \frac{\partial}{\partial \varphi}u_\varphi = 0,
$$

(3.1)

where $\mathbf{v} = (u_r, u_z, u_\varphi)^T$. Here $u_r$, $u_z$, $u_\varphi$ are the velocity components in $r$, $z$, and $\varphi$ directions respectively. In the axisymmetric case we have $u_\varphi = 0$, and (3.1) simplifies to

$$
\frac{1}{r} \frac{\partial}{\partial r}(ru_r) + \frac{\partial}{\partial z}u_z = 0.
$$

(3.2)

For $(u_r, u_z)^T$ one can define a stream function $\psi$ such that
This gives a system of ordinary differential equations

\[
\begin{align*}
\dot{u}_r &= - \frac{1}{r} \frac{\partial \psi}{\partial z}, \\
\dot{u}_z &= \frac{1}{r} \frac{\partial \psi}{\partial r}.
\end{align*}
\] (3.3)

Clearly, (3.4) is not a Hamiltonian system

\[
\frac{\partial}{\partial z} \frac{dr}{dt} + \frac{\partial}{\partial r} \frac{dz}{dt} \neq 0.
\] (3.5)

We can, however, find a transformation of variables which does lead to a Hamiltonian form, viz.

\[
x := \frac{1}{2} r^2, \quad y := z.
\] (3.6)

Then it is easy to see that

\[
\begin{align*}
\frac{dx}{dt} &= \sqrt{2x} \, u_r(\sqrt{2x}, y), \\
\frac{dy}{dt} &= u_z(\sqrt{2x}, y).
\end{align*}
\] (3.7)

which is a Hamiltonian system with respect to \(x\) and \(y\). Using (3.3), (3.6) we can derive an equivalent formulation

\[
\begin{align*}
\frac{dx}{dt} &= \sqrt{2x} \, u_r(\sqrt{2x}, y), \\
\frac{dy}{dt} &= u_z(\sqrt{2x}, y).
\end{align*}
\] (3.8)

Consider now the following system of ordinary differential equations (which is equivalent to (3.4))

\[
\begin{align*}
\dot{r} &= u_r(r, z), \\
\dot{z} &= u_z(r, z).
\end{align*}
\] (3.9)

Direct application of the midpoint rule to (3.9) gives

\[
\begin{align*}
\Delta t^{k+1} &= r^k + \Delta t \, u_r \left( \frac{r^k + r^{k+1}}{2}, \frac{z^k + z^{k+1}}{2} \right), \\
\Delta t^{k+1} &= z^k + \Delta t \, u_z \left( \frac{r^k + r^{k+1}}{2}, \frac{z^k + z^{k+1}}{2} \right).
\end{align*}
\] (3.10)
On the other hand, if we apply the midpoint rule to (3.8) we obtain

\[
\begin{aligned}
x^{k+1} &= x^k + \Delta t \sqrt{x^k + x^{k+1}} u_r \left( \sqrt{x^k + x^{k+1}}, \frac{y^k + y^{k+1}}{2} \right), \\
y^{k+1} &= y^k + \Delta t \; u_z \left( \sqrt{x^k + x^{k+1}}, \frac{y^k + y^{k+1}}{2} \right).
\end{aligned}
\]  

(3.11)

Since (3.10) and (3.11) are implicit we may e.g. employ a predictor-corrector method to find a solution. Of course, this requires the problem to be not stiff, which we therefore assume here. We use Euler forward as a predictor. For (3.8) this leads to

\[
\begin{aligned}
x^{k+1} &= x^k + \Delta t \sqrt{2x^k} u_r (\sqrt{2x^k}, y^k), \\
y^{k+1} &= y^k + \Delta t \; u_z (\sqrt{2x^k}, y^k).
\end{aligned}
\]  

(3.12)

A corrector then iterates on \( x^{k+1} \) in (3.11). Let us illustrate these methods by two examples.

Example 3.1. Consider an axisymmetric velocity field given by

\[
\begin{aligned}
\frac{dr}{dt} &= -\pi r, \\
\frac{dz}{dt} &= 2\pi z.
\end{aligned}
\]  

(3.13)

These equations can simply be solved to give

\[
\begin{aligned}
r(t) &= r(0) e^{-\pi t}, \\
z(t) &= z(0) e^{2\pi t}.
\end{aligned}
\]  

(3.14)

In particular let the initial domain be a cylinder with radius \( r = 1 \) and height \( h = \pi \), being the initial values of functions \( r(t) \) and \( z(t) \) respectively. Then it can be seen that the volume of the body \( V(t) := \pi r(t)^2 z(t) \) remains constant and maintains a cylindrical form. Indeed, the points at the top of the cylinder (see Figure 3.1) all move with the same speed downwards. Those at the bottom have vertical velocity equal to zero and those at the cylinder surface all have the same radial velocity. One can see that the geometry of the cylinder is defined by the motion of the point \( P(t) \), which has initial value \( P(0) := (r(0), z(0))^T \).

As for solving the problem numerically, a direct application of the midpoint rule (see (3.10)) to (3.13) gives

\[
\begin{aligned}
r^{k+1} &= r^k - \frac{\pi}{2} \Delta t (r^k + r^{k+1}), \\
z^{k+1} &= z^k + \Delta t \; 2\pi (z^k + z^{k+1}).
\end{aligned}
\]  

(3.15)

So that we find

\[
r^{k+1} = \frac{1 - \Delta t \; \pi/2}{1 + \Delta t \; \pi/2} r^k, \quad z^{k+1} = \frac{1 - \Delta t \; \pi}{1 + \Delta t \; \pi} z^k.
\]  

(3.16)

Hence
Figure 3.1: Cylinder evolution in time (Example 3.1).

\[
\left[ \frac{1}{2} \left( r^{k+1} \right)^2 z^{k+1} \right] = \left( \frac{1 - \Delta t \pi/2}{1 + \Delta t \pi/2} \right)^2 \frac{1 + \Delta t \pi}{1 - \Delta t \pi} \left[ \frac{1}{2} \left( r^k \right)^2 z^k \right]. \tag{3.17}
\]

From (3.17) we clearly see that we do not have conservation of volume.

Now we associate a Hamiltonian \( \psi(r, z) = \pi r^2 z \) to the point \( P(t) \). Clearly, it satisfies the form in (3.4). Using (3.11) we obtain

\[
\begin{align*}
  x^{k+1} &= x^k - \Delta t \pi (x^k + x^{k+1}), \\
  y^{k+1} &= y^k + \Delta t \pi (y^k + y^{k+1}).
\end{align*} \tag{3.18}
\]

Consequently we have

\[
\left[ \frac{1}{2} \left( r^{k+1} \right)^2 z^{k+1} \right] = \frac{1 - \Delta t \pi}{1 + \Delta t \pi} \cdot \frac{1 + \Delta t \pi}{1 - \Delta t \pi} \left[ \frac{1}{2} \left( r^k \right)^2 z^k \right]. \tag{3.19}
\]

Hence this method conserves the volume numerically.

We have performed a numerical simulation of \( P(t) \), a point at the top edge of the cylinder (see Figure 3.1a), for \( t \in [0, 0.2] \). This gives the values for \( r(t) \) and \( z(t) \) and thus we can find an estimate of the volume as well. In Figure 3.2 we have plotted the error, i.e. the difference between
Figure 3.2: Volume error graphs for different number of mid-point correction steps (Example 3.1).

exact and numerical volume as a function of $t$ for various values of $N_c$, the number of correction steps. For $N_c = 8$ we appear to have full accuracy (up to round-off error).

The next example will demonstrate the idea for a non-linear problem.

**Example 3.2.** Consider a cylindrically symmetric three dimensional velocity field

$$
\begin{align*}
    u_r &= -\frac{1}{8}r^2 \cos z, \\
    u_z &= \frac{1}{2}r^2 \sin z.
\end{align*}
$$

Since (3.2) is satisfied, the velocity field above is divergence free. Rewriting $r, z$ in terms of $x, y$ (see (3.6)) gives
This system is a Hamiltonian system. Indeed, one can easily find the expression for the Hamiltonian itself

\[
\psi(x, y) = \frac{1}{2} x^2 \sin y.
\]  

(3.22)

Figure 3.3: Cylinder evolution in time (Example 3.2).

In Figure 3.3a we have drawn a typical cylinder with radius 1 and height \( \pi \). The initial position of the cylinder’s upper and lower planes correspond to \( z = \pi \) and \( z = 0 \) respectively. Clearly, the relative positions of “points” on the cylinder will not change during the evolution. Note that the velocity component in the \( z \)-direction is proportional to \( \sin z \) and stays 0 for \( z = 0, \pi \). The volume of the body at time \( t \) can be represented by the following integral

\[
\frac{\pi}{3} \int_0^\pi (\hat{r}^2(z) + \hat{r}(z) + 1) \, dz,
\]  

(3.23)

where \( \hat{r}(z) \) describes the geometry of an axisymmetric body. The evolution of the resulting surface is depicted in Figure 3.3.
As was illustrated in the first example, conservation of volume depends on the number of correction steps. However, here we have a more complicated surface requiring numerical integration. Therefore we introduce another parameter, $N_h$, say, that indicates the number of intervals used in an equispaced trapezoidal rule. We like to point out that this $N_h$ is not relevant for our method as such (and indeed a higher order quadrature formula would do a much better job). Yet it is interesting to see how the accuracy improves by increasing $N_h$, see Figure 3.4. Note that the trapezoidal method is second order (in space!) and is apparently dictating the overall accuracy.

![Graphs](image)

Figure 3.4: Volume error graphs for different number of integration intervals (Example 3.2).

### 4 Hamiltonians for 3-D Axisymmetric Cases: Spherical Coordinates

Another coordinate system that is useful in symmetry considerations, is given by spherical coordinates, say $r, \theta, \varphi$ for radius, azimuth, and zenith respectively. We then find

$$\nabla \cdot \mathbf{v} = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 u_r) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta u_\theta) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \varphi} (u_\varphi) = 0. \quad (4.1)$$
In the axisymmetric case, \( u_\phi = 0 \), so we find
\[
\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 u_r) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta \ u_\theta) = 0. \tag{4.2}
\]

For (4.2) we can find a stream function \( \psi \) with
\[
\begin{align*}
  u_r &= \frac{1}{r^2 \sin \theta} \frac{\partial \psi}{\partial \theta}, \\
  u_\theta &= -\frac{1}{r \sin \theta} \frac{\partial \psi}{\partial r},
\end{align*} \tag{4.3}
\]

where one should note that
\[
  u_r = \frac{dr}{dt}, \quad u_\theta = r \frac{d\theta}{dt}. \tag{4.4}
\]

Hence, similarly to (3.4), we obtain a system of ordinary differential equations
\[
\begin{align*}
  \frac{dr}{dt} &= \frac{1}{r^2 \sin \theta} \frac{\partial \psi}{\partial \theta}, \\
  \frac{d\theta}{dt} &= -\frac{1}{r \sin \theta} \frac{\partial \psi}{\partial r}.
\end{align*} \tag{4.5}
\]

Clearly, (4.5) is not a Hamiltonian system (see (2.6)). With some trial and error we find the proper transformation for putting (4.5) in Hamiltonian form, viz.
\[
x := r^3/3, \quad y := \cos \theta. \tag{4.6}
\]

We derive the following Hamiltonian system in \( x, y \)
\[
\begin{align*}
  \frac{dx}{dt} &= r^2 \frac{dr}{dt} = \frac{1}{\sin \theta} \frac{\partial \psi}{\partial \theta} = -\frac{\partial \psi}{\partial y}, \\
  \frac{dy}{dt} &= -\sin \theta \frac{d\theta}{dt} = \frac{1}{r^2} \frac{\partial \psi}{\partial r} = \frac{\partial \psi}{\partial x}.
\end{align*} \tag{4.7}
\]

As a consequence we have to use the following form to retain volume conservation when solving the evolution equations, given the velocities \( u_r \) and \( u_\theta \),
\[
\begin{align*}
  \frac{dx}{dt} &= (3x)^{2/3} u_r((3x)^{1/3}, \arccos y), \\
  \frac{dy}{dt} &= \sqrt{1 - y^2} (3x)^{1/3} u_\theta((3x)^{1/3}, \arccos y). \tag{4.8}
\end{align*}
\]

Of course, we have to be careful with these transformations since they are meromorphic. We illustrate the idea in the next example.

**Example 4.1.** Consider a sphere with radius 1 in a uniform stream. If we assume that the velocity \( v = 0 \) on the boundary of the sphere and goes to some fixed value, 1 in the radial direction say, if \( r \to \infty \). Then it is well known (see [10]) that the Stokes equation (which describes viscous flow for incompressible fluids) can be solved exactly, if one moreover prescribes the pressure for \( r \) at infinity. The resulting stream function reads
\[ \psi = \left( \frac{1}{2} r^2 - \frac{3}{4} r + \frac{1}{4r} \right) \sin^2 \theta. \]  \hspace{1cm} (4.9)

The velocities are given by

\[ \begin{align*}
    u_r &= \left( 1 - \frac{3}{2r} + \frac{1}{2r^2} \right) \cos \theta \\
    u_\theta &= \left( -1 + \frac{3}{4r} + \frac{1}{4r^3} \right) \sin \theta.
\end{align*} \]  \hspace{1cm} (4.10)

If we transform this in \( x, y \) coordinates using (4.6), we obtain (cf. (4.8))

\[ \begin{align*}
    \frac{dx}{dt} &= \left( (3x)^{2/3} - \frac{3}{2} (3x)^{1/3} \right) \frac{1}{2} + \frac{1}{2(3x)^{1/3}} y \\
    \frac{dy}{dt} &= \left( - (3x)^{1/3} + \frac{3}{4} (3x)^{2/3} + \frac{1}{4(3x)^{4/3}} \right) \left( 1 - y^2 \right). \hspace{1cm} (4.11)
\end{align*} \]

Figure 4.1: Motion of the Stokes flow (Example 4.1).

In Figure 4.1 we have depicted the evolution of a hollow cylindrical body moving past the sphere with \( \Delta t = 10^{-1} \). We performed the trapezoidal rule for integration, like in Example 3.2. As can be seen in Figure 4.2 the error decreases quadratically, i.e. \( \sim \left( \frac{1}{N_h} \right)^2 \), where \( N_h \) is the number of spatial intervals for this integration. Again we can conclude that the mass is numerically conserved, to high accuracy at least.

5 Hamiltonians for 3-D Spherically Symmetric Problems

Quite different from the situation discussed in foregoing two sections is the evolution of a patch on a sphere. Here we have a 2-D problem, but as before, the stream function is not a Hamiltonian without transformation of the variables.

Recall the divergence (4.2). If we have spherical symmetry then \( \partial / \partial r = 0 \). Hence we have (\( r \) being constant)

\[ \nabla \cdot \mathbf{v} = \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (\sin \theta u_\theta) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} u_\phi = 0. \]  \hspace{1cm} (5.1)
Figure 4.2: Volume error graphs for different number of discretisation intervals (Example 4.1).

For (5.1) we can define a stream function $\psi$ with

$$
\begin{cases}
  u_\theta = \frac{1}{\sin \theta} \frac{\partial \psi}{\partial \theta'}, \\
  u_\varphi = -\frac{\partial \psi}{\partial \varphi'}
\end{cases}
$$

(5.2)

Note that now

$$
u_\theta = r \frac{d \theta}{dt}, \quad u_\varphi = r \sin \theta \frac{d \varphi}{dt}.
$$

(5.3)

Since $\frac{\partial}{\partial \theta'} u_\theta + \frac{\partial}{\partial \varphi'} u_\varphi \neq 0$, we use the transformation

$$
x := r \cos \theta, \quad y := \varphi.
$$

(5.4)

Then (5.2) can be reformulated in terms of $x$ and $y$.
\[
\begin{align*}
\frac{dx}{dt} &= -r \sin \theta \frac{d\theta}{dt} = -\sin \theta \frac{u_\varphi}{r}, \\
\frac{dy}{dt} &= \frac{1}{r \sin \theta} \frac{u_\varphi}{r} = \frac{1}{r \sin \theta} \frac{\partial \psi}{\partial y}.
\end{align*}
\]

So in fact one should use the following conservative formulation

\[
\begin{align*}
\frac{dx}{dt} &= -\sqrt{1 - \frac{x^2}{r^2}} u_\varphi(\arccos \frac{x}{r}, y), \\
\frac{dy}{dt} &= \frac{1}{r} \sqrt{1 - \frac{x^2}{r^2}} u_\varphi(\arccos \frac{x}{r}, y).
\end{align*}
\]

Again, one should take care and possibly consider separate (though connected) intervals to overcome problems of multivalued functions or singularities.

**Example 5.1.** Consider a sphere with radius \( r = 1 \) and 4 points on a sphere that are connected by geodesic; the enclosure forms a patch. We have an initial patch (see Figure 5.1a) of which the evolution is defined by the following system of ODE

\[
\begin{align*}
\frac{d\theta}{dt} &= \frac{1}{\sin \theta} \varphi, \\
\frac{d\varphi}{dt} &= \cos \theta.
\end{align*}
\]

Since (5.1) is satisfied, the velocity field defined by (5.7) is divergence free. If we take \( \psi(\theta, \varphi) := \frac{1}{4}(\cos^2 \theta + \varphi^2) \), then \( \psi \) is clearly a conserved quantity as a function of \( \theta \) and \( \varphi \). Note that we obtain in transformed coordinates

\[
\begin{align*}
\frac{dx}{dt} &= -y, \\
\frac{dy}{dt} &= x.
\end{align*}
\]

In Figure 5.1 we have depicted the evolution of the patch using the midpoint rule for \( \Delta t = 10^{-1} \) and \( t \in [0, 10] \).

![Figure 5.1: Evolution of the patch on a sphere (Example 5.1).](image)
Since the numerical results are very accurate (cf. Example 3.1) we have also displayed the final position for a number of different time steps $\Delta t$ for an evolution on the interval $[0, 10]$ (see Figure 5.2). The area is still nicely conserved, although the patches are more out of phase, the larger $\Delta t$ becomes. The latter fact is, of course the result of discretisation errors.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure52.png}
\caption{Resulting patch for different time steps at $t = 10$ (Example 5.1).}
\end{figure}

6 Midpoint Rule for Autonomous Velocity Fields

So far we have assumed that $v$ was available in explicit form. Of course, in practice the velocity is computed from continuity and momentum equations numerically. We may assume that this has been done to some degree of accuracy, e.g. by a finite element method (cf. [12]). The question is now how to use the midpoint rule, as we do not have values for the velocities at midpoints, even less at the unknown end points. Since (1.1) is an ODE we could still formally use Euler forward to predict the next time level position, in fact adopting a Lagrangian point of view. We then still have the formal problem that a correction by the midpoint rule would be at best an approximate real midpoint step, as we do not know exact trajectories (of the ODE!). Below we work out an alternative method which both avoids iteration and problems at intermediate points; the only cost is some interpolation (including errors resulting from this).

We shall first sketch the idea for a scalar equation; so consider

$$\frac{dx}{dt} = v(x), \quad t \in [0, T]. \quad (6.1)$$

Though dealing with an ODE, we now like to see $x(t)$ as a element of a flow, i.e. a compactum $I(t)$ moving on the x-axis in time. Let $x(0) \in I(0)$, then $x(t) \in I(t)$. So with $x^0 = x(0)$ we obtain $x^k$ by numerical integration with $\Delta t$ as step size. If we have a set of points $x_i(0), \ i = 1, \ldots, N$, with $x_i(0) \in I(0)$ then defining $x_i^k$ as the numerical approximant of $x_i(t^k)$ for $i = 1, \ldots, N$, we can find an approximation of $I(t^k)$ by interpolating on the values $x_i^k$.

The idea is to bypass the implicitness of the midpoint rule, by employing the autonomy of (6.1). For this we realize that the midpoint rule on $(t^k, t^{k+\frac{1}{2}})$ coincides with the Euler backward method applied on that interval, see Figure 6.1a. Therefore, if we would know the direction field at $t^{k+\frac{1}{2}}$, we could do a “forward” step in negative time direction and obtain values at $t^k$, $x_i^k$ say, see Figure 6.1b. Any $x_i^k$ can be seen as a certain weighted average of those points, e.g. the point $x_0^k$ can be found from $x_1^k$ and $x_2^k$ by linear interpolation (see Figure 6.1c). This in turn is then used with
the same weights for the $v$-values at $t^{k+\frac{1}{2}}$ to obtain an approximate $v(x_i^{k+\frac{1}{2}})$. The nice thing about autonomous ODE is that the direction field is constant in time. So we simply use the $v$-values at $t_i^k$ for those at $t_i^{k+\frac{1}{2}}$. Of course, one can use higher order interpolation too, giving a more accurate computation of $v(x_i^{k+\frac{1}{2}})$ (within accuracy bounds set by the local discretisation error).

The final step now is to compute $x_i^{k+1}$ as

$$x_i^{k+1} = x_i^k + \Delta t v(x_i^{k+\frac{1}{2}}), \quad i = 1, \ldots, N. \quad (6.2)$$

Note that $v(x_i^{k+\frac{1}{2}})$ is not known exactly, being the price for employing interpolation. Yet, the results are remarkably good, see examples below. The set of points $x_i^k$ may be reshuffled, all depending on how the flow moves. A further discussion of this is outside the scope of this paper and will be dealt with elsewhere.

The method above can be applied to two (and three) dimensional problems as well. Consider an autonomous Hamiltonian system for $\mathbf{x} = (x, y)^T$

$$\frac{d\mathbf{x}}{dt} = \mathbf{v}(\mathbf{x}), \quad t \in [0, T], \quad (6.3)$$

where $\mathbf{v}(\mathbf{x}) = (u_x(x, y), u_y(x, y))^T$. The integration rule for a particular point $\mathbf{x}_i$ reads

$$x_i^{k+1} = x_i^k + \Delta t v(x_i^{k+\frac{1}{2}}). \quad (6.4)$$

Figure 6.1: The method.
We define $\tilde{x}_i^{k+\frac{1}{2}}$ as the result of shifting of $x_i^k$ over $\frac{1}{2} \Delta t$, and because the system is autonomous we have

$$v(x_i^{k+\frac{1}{2}}) = v(x_i^k). \tag{6.5}$$

We first employ linear interpolation to approximate the velocity at $x_i^{k+\frac{1}{2}}$. So we choose some $x_j^{k+\frac{1}{2}}, j = 1, 2, 3$. By “integrating backwards” we obtain

$$\tilde{x}_j^k = x_j^{k+\frac{1}{2}} - \frac{1}{2} \Delta t v(x_j^{k+\frac{1}{2}}), \quad j = 1, 2, 3. \tag{6.6}$$

We now use the thus obtained $\tilde{x}_j^k, j = 1, 2, 3,$ as interpolation points at $t^k$ and $v(x_j^{k+\frac{1}{2}}), j = 1, 2, 3,$ as values, to find a vector interpolation polynomial

$$g(x) = \left( \begin{array}{c} a_x x + b_x y + c_x \\ a_y x + b_y y + c_y \end{array} \right), \tag{6.7}$$

such that $g(x_i^k) = v(x_i^{k+\frac{1}{2}}), j = 1, 2, 3$. The interpolation of the velocity at $x_i^{k+\frac{1}{2}}$ is then found as

$$v(x_i^{k+\frac{1}{2}}) = g(x_i^k). \tag{6.8}$$

In order to use a higher order interpolation one should choose more points $\tilde{x}_j^{k+\frac{1}{2}},$ say $j = 1, \ldots, n$. For $n = 6$, for example, this could be quadratic interpolation and $g$ will have the following form

$$g(x) = \left( \begin{array}{c} a_x x^2 + b_x y^2 + c_x x y + d_x x + e_x y + f_x \\ a_y x^2 + b_y y^2 + c_y x y + d_y x + e_y y + f_y \end{array} \right). \tag{6.9}$$

To illustrate the method above we give the two examples. Both deal with 3-D cases where symmetry allows for a suitable Hamiltonian formulation. The first example is just to demonstrate the quality of the method; therefore it uses a given vector field $v$ (as in Example 3.2). The second example employs a Finite Element method to solve a series of Stokes problems for obtaining the velocity field.

**Example 6.1.** In this example we consider the same ODE as Example 3.2, i.e. an axisymmetric problem where the velocity field is given by (see (3.20))

$$\begin{cases} u_r = -\frac{1}{8} r^4 \cos z, \\ u_z = \frac{1}{2} r^2 \sin z. \end{cases} \tag{6.10}$$

We now let the initial domain be an ellipsoid with principle axis in the $r$ and $z$ direction equal to 2 and 1 respectively. Clearly, for computational purposes we employ the formulation (3.21), where the initial domain is a transformed quarter of an ellipse. A graphical description of its evolution from $t = 0$ to $t = 0.3$ is given in Figure 6.2. For the numerical experiments we choose the time step as $\Delta t = 10^{-2}$. The number of points at the boundary is taken equal to $N_h = 2^6$. For the time stepping we use the implicit midpoint rule in the setting outlined above. First we employ linear interpolation. In Figure 6.3a we have depicted the difference between the exact volume of the body and the volume found by the numerical approximation method. We remark that the error is proportional to $t$. This can be seen as the cumulative interpolation error in $v$. Note that at each time step the contribution of the interpolation to the local error equals the interpolation error.
Figure 6.2: Evolution of an ellipse (Example 6.1).

This is confirmed by Figure 6.3b, where we have displayed the error when quadratic interpolation is used; the error is still linear in $t$. Actually we see that the error drops by two decades, showing that it is a result of interpolation indeed (so the discretisation errors from the midpoint rule do not show up). The high accuracy in both cases (much more than to be expected from $O(\Delta t^2)$) confirms that we have effectively “numerical conservation”.

Example 6.2. This example illustrates how the algorithm can be applied when $v$ is not known explicitly. Note that in all previous examples the velocity field and the stream function were known analytically, through the whole time interval. We now use velocities which are computed numerically.

Consider the motion of a viscous axisymmetric body driven by the surface tension. This problem can be described by the Stokes equations (see [11])

$$\nabla \cdot \sigma = 0,$$
$$\nabla \cdot \mathbf{v} = 0,$$  \hspace{1cm} (6.11)

where $\sigma = -pI + \eta(\nabla \mathbf{v} + (\nabla \mathbf{v})^T)$ is the stress tensor. Here $\mathbf{v}$ is the velocity of the fluid, and $p$ is the pressure. Since we have axisymmetry we can take $\mathbf{v} = (u_r(r, z), u_z(r, z))^T$.

Let us take an ellipsoid as initial value for the body, with principle axis in $r$ and $z$ direction equal to 2 and 1 respectively. In fact, one can employ the symmetry to let the initial computational
domain $\Omega_0$ be a quarter of an ellipse (cf. Figure 6.4a). Clearly, the boundary of the domain $\Gamma$ consists of three parts $\Gamma = \Gamma_{Or} \cup \Gamma_{Os} \cup \Gamma_s$. Therefore we have three types of boundary conditions for every part of the boundary. For $x \in \Gamma_{Or} \cup \Gamma_{Os}$ we have symmetric boundary conditions which read as follows

\begin{align}
  v \cdot n &= 0, \\
  \sigma n \cdot t &= 0, 
\end{align}

(6.12)

where $n$ is the outward normal and $t$ is the tangent to the boundary.

For $x \in \Gamma_s$ we use the so called surface tension boundary conditions (see [11]) which can be written as

\begin{equation}
  \sigma n = -k(s) n. 
\end{equation}

(6.13)

Here $k(s)$ is the curvature of the boundary.

We use finite elements to discretise the problem (see [12]); they give a solution with second order errors (in the mesh size). The resulting system of linear equations has the following block structure

\begin{equation}
  \begin{pmatrix}
    A & B \\
    B^T & 0
  \end{pmatrix}
  \begin{pmatrix}
    u \\
    p
  \end{pmatrix}
  =
  \begin{pmatrix}
    f_1 \\
    f_2
  \end{pmatrix},
\end{equation}

(6.14)

where $A$ is a symmetric positive definite matrix and $u, p$ are the vectors of unknown velocity and pressure respectively. The system can e.g. be solved using a Schur complement method, see [12]. This requires the matrix $A$ to be easily invertible (unless an iterative procedure is going to be used). For this we obtain a complete Cholesky factor of $A$, after permuting the matrix according to a minimum degree reordering (see [9]).

Once we have boundary data (in particular the free boundary) we can use them to obtain the
Figure 6.4: Evolution of the Stokes flow driven by the surface tension in time (Example 6.2).

velocity field at a certain time point. And consequently in a time stepping method. For the latter we have to solve (3.9). However, we use to (3.8) instead, which is a Hamiltonian system.

In Figure 6.5 we have depicted the evolution computed by employing the implicit midpoint rule with with $\Delta t = 10^{-2}$ and the algorithm outlined above (see (6.4)-(6.8)) with various values of the number of discretisation intervals at the boundary, $N_h$. In Figure 6.5 one can see that the accuracy of the computed area is much higher than the discretisation error and quadratic in the grid size. Since linear interpolation gives second order accuracy, quadratic interpolation does not improve the accuracy here, as the Stokes solver is second order. This is due to the fact that the velocity field is not known exactly and therefore the discretisation error (from FEM solver) limits the volume preservation.
Figure 6.5: Area error graphs for the midpoint rule with fixed time step and different mesh sizes: $\Delta t = 10^{-2}$, $N_h = 2^7$ (Example 6.2).

References


