Employing Hamiltonian formulations for numerical mass conservation

Employing Hamiltonian Formulations for Numerical Mass Conservation

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

1 Introduction

An important concept in physical applications is conservation. In this paper we are in particular interested in how we can conserve mass in fluid flow. The mass conservation for an incompressible fluid reads

$$\operatorname{div} \mathbf{v} = 0,$$

where $\mathbf{v}$ is the velocity of the fluid. In a two dimensional situation one can easily associate $\mathbf{v}$ to a stream function, a Hamiltonian which asks for special numerical treatment in order to have conservation. If we have a three dimensional problem such a formulation is not possible. Yet, in cases of symmetry we can often reformulate the problem as a two dimensional problem. With some appropriate change of variables this then results in a (Hamiltonian) stream function.

This paper is built up as follows. In Section 2 we consider the relationship between conservation, the stream function as a Hamiltonian and how this can be applied in a three dimensional axisymmetric case. Then in Section 3 we briefly describe the use of the midpoint rule, a simplectic numerical method that conserves quantities in a time stepping procedure. In Section 4 we give two examples to illustrate this conservation. Finally, in Section 5 we consider an application of the method in a practical simulation: the pressing of glass in a mould.

2 Conservation and Hamiltonian Systems

If we have an incompressible fluid with density ρ, moving with velocity $\mathbf{v}$ then the conservation of mass can be expressed as

$$\nabla \cdot \rho \mathbf{v} = 0.$$

Since ρ is constant this simplifies to

$$\nabla \cdot \mathbf{v} = 0. \tag{2.1}$$

This law implies that a certain volume, $V^{xy}(t)$ say, remains constant, i.e. is conserved. For a two dimensional flow this has an interesting consequence. Let us denote a vector $\mathbf{x} \in V^{xy}(t)$ as

$$\mathbf{x} = (x, y)^T, \tag{2.2}$$

and the velocities in x and y direction by u and v respectively

$$\mathbf{v}(x, y) = \big(u_x(x, y),\ u_y(x, y)\big)^T. \tag{2.3}$$

Then (2.1) implies

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

As is well-known we can associate a stream function $\phi^{xy}(x, y)$ to (2.1) with

$$u_x = -\frac{\partial \phi^{xy}}{\partial y}, \quad u_y = \frac{\partial \phi^{xy}}{\partial x}. \tag{2.5}$$

In other words we have a simple Hamiltonian system

$$\begin{cases} \dfrac{d}{dt}x &= -\dfrac{\partial \phi^{xy}}{\partial y} \\ \dfrac{d}{dt}y &= \dfrac{\partial \phi^{xy}}{\partial x}. \end{cases} \tag{2.6}$$

The stream function ϕ^{xy} is thus a Hamiltonian associated to $\mathbf{v}$. General Hamiltonian systems have a a number of nice properties. One if these is that they are volume preserving, being a generalization of what we already observed from our conservation law. Unfortunately, they typically have an even dimension, so that we not can hope to find an analogue in a three dimensional case (see [1]). However, for special situations in three dimensions we can still find a stream function which turns out to be a Hamiltonian indeed. In particular, consider an axisymmetric flow. If we let r denote the radial coordinate and z the azimuthal coordinate then a typical volume is given by

$$V^{rz} = 2\pi \int_{V^{rz}} r\, dr dz.$$

In cylindrical coordinates the continuity equation (2.1) then reads

$$\frac{1}{r}\frac{\partial}{\partial r}u_r + \frac{\partial}{\partial z}u_z = 0, \quad r > 0, \tag{2.7}$$

where $\mathbf{v}(r, z) = (u_r(r, z), u_z(r, z))$ is the velocity of the fluid. Writing

$$x := \frac{1}{2}r^2, \quad y := z, \tag{2.8}$$

we see that (2.7) can be rewritten in the form (2.4), where $u_x(x,y) \equiv u_r(r,z)$ and $u_y(x,y) \equiv u_z(r,z)$. Hence we can associate to (2.7) a stream function $\phi^{rz}(r^2/2, z)$ with

$$u_r = -\frac{\partial \phi^{rz}}{\partial y} = -\frac{\partial \phi^{rz}}{\partial z}, \quad u_z = \frac{\partial \phi^{rz}}{\partial x} = \frac{1}{r}\frac{\partial \phi^{rz}}{\partial r}. \tag{2.9}$$

Clearly we essentially have a two dimensional situation again and from (2.6) and (2.8) we deduce the Hamiltonian system for the cylindrically symmetric case

$$\begin{cases} \dfrac{d}{dt}\left(\dfrac{r^2}{2}\right) &= -\dfrac{\partial \phi^{rz}}{\partial z} \\ \dfrac{d}{dt}z &= \dfrac{\partial \phi^{rz}}{\partial \left(\dfrac{r^2}{2}\right)}. \end{cases} \tag{2.10}$$

One may rewrite (2.10) as

$$\begin{cases} \dfrac{d}{dt}r &= -\dfrac{1}{r}\dfrac{\partial \phi^{rz}}{\partial z} \\ \dfrac{d}{dt}z &= \dfrac{1}{r}\dfrac{\partial \phi^{rz}}{\partial r}, \end{cases} \tag{2.11}$$

However, the latter is not in conservative form, i.e. $\dfrac{\partial}{\partial z}\dfrac{dr}{dt} + \dfrac{\partial}{\partial r}\dfrac{dz}{dt} \neq 0$.

Note that we can associate to $V^{rz}(t)$ a volume in $\mathbb{R}^2$, V^{xy} say, with

$$V^{rz}(t) = 2\pi \int_{V^{rz}(t)} r dr dz = 2\pi V^{xy}(t) = 2\pi \int_{V^{xy}(t)} dx dy. \tag{2.12}$$

Clearly, the three dimensional volume V^{rz} is conserved as long as the two dimensional volume V^{xy} associated to (2.8) is conserved.

3 Numerical Symplectic Schemes

If we use a numerical method to solve a problem in fluid mechanics we should preferably choose a method that preserves physically relevant properties. This requirement has less to do with accuracy arguments as such. Indeed, a quantity like the total mass that should be conserved during the evolution of the motion of the fluid, may be preserved more accurately if a mesh width in a numerical scheme is made smaller. However, we rather would like to use a method which preserves the mass, irrespective of the mesh. In terms of the setting in Section 2 this carries over to volume preservation. Fortunately, there exists a number of numerical methods that have this property for Hamiltonian problems. For a more detailed overview of such so called symplectic

schemes, see [1]. In this paper we will be satisfied with studying the implicit midpoint rule, which for the system

$$\begin{cases} \dfrac{dx}{dt} &= u_x \\ \\ \dfrac{dy}{dt} &= u_y, \end{cases} \tag{3.1}$$

reads

$$\begin{cases} x^{k+1} &= x^k + \Delta t\, u_x(\mathbf{q}^k(x,y)) \\ \\ y^{k+1} &= y^k + \Delta t\, u_y(\mathbf{q}^k(x,y)), \end{cases} \tag{3.2}$$

where $\mathbf{q}^k(x,y) := \left((x^k + x^{k+1})/2,\, (y^k + y^{k+1})/2\right)^T$.

Note that this method is second order in Δt. For applying (3.2) to the Hamiltonian system (2.6) it is sufficient to know u_x and u_y. A time stepping for a linear system (2.6) will give a conserved flow volume, see [1]. For nonlinear systems this is not necessary so, although it still often produces "nearly conserved volumes" (see [1]).

For axisymmetric flows we can now simply apply (3.2) to (2.11). Taking into account (2.9) this gives the following simplectic integration scheme for an axisymmetric flow

$$\begin{cases} r^{k+1} &= r^k + \dfrac{2\Delta t}{r^k + r^{k+1}}\, u_r(\mathbf{q}^k(r,z)) \\ \\ z^{k+1} &= z^k + \dfrac{2\Delta t}{r^k + r^{k+1}}\, u_z(\mathbf{q}^k(r,z)). \end{cases} \tag{3.3}$$

Since $\mathbf{v}$ may involve a complicated computation, we use a predictor-corrector technique, with Euler forward as a predictor, see [3]. Let us denote the predictor value by $(r_0^{k+1}, z_0^{k+1})^T$ and the corrector values by $(r_j^{k+1}, z_j^{k+1})^T,\ j \geq 1$, then we have for (3.3)

$$\begin{cases} r_{j+1}^{k+1} &= r^k + \dfrac{2\Delta t}{r^k + r_j^{k+1}} u_r(\mathbf{q}_j^k(r,z)) \\ \\ z_{j+1}^{k+1} &= z^k + \dfrac{2\Delta t}{r^k + r_j^{k+1}} u_z(\mathbf{q}_j^k(r,z)), \end{cases} \tag{3.4}$$

where $\mathbf{q}_j^k(x,y) := \left((r^k + r_j^{k+1})/2,\, (z^k + z_j^k)/2\right)^T$.

An alternative formulation for (3.3) is to use $r^2/2$ as an unknown, i.e. applying (3.2) to (2.10). Using the correspondence between (u_x, u_y) and (u_r, u_z) we then obtain

$$\begin{cases} \dfrac{1}{2} r^{k+1^2} &= \dfrac{1}{2} r^{k^2} + \Delta t\, u_x(\mathbf{q}^k(r^2/2, z)) \\ \\ z^{k+1} &= z^k + \Delta t\, u_y(\mathbf{q}^k(r^2/2, z)), \end{cases} \tag{3.5}$$

Note that for (3.5) we obtain the corrector (3.6)

$$\begin{cases} \frac{1}{2}r_{j+1}^{k+1\,2} &= \frac{1}{2}r^{k\,2} + \Delta t u_x(\mathbf{q}_j^k(r^2/2, z)) \\ z_{j+1}^{k+1} &= z^k + \Delta t u_y(\mathbf{q}_j^k(r^2/2, z)). \end{cases} \tag{3.6}$$

After N steps we stop the iteration and define

$$r^{k+1} := r_N^{k+1}, \quad z^{k+1} := z_N^{k+1}. \tag{3.7}$$

Below we shall illustrate these schemes.

4 Examples

Example 1. Consider an axisymmetrical velocity field $D(t) \in \mathbb{R}^3$, given by

$$\begin{cases} u_r &= -\pi r, \\ u_z &= 2\pi z. \end{cases} \tag{4.1}$$

These equations can simply be solved to give

$$\begin{cases} r(t) &= r(0)e^{-\pi t}, \\ z(t) &= z(0)e^{2\pi t}. \end{cases} \tag{4.2}$$

In particular let $D(0)$ be a cylinder with radius $R(0) = R_0$ and height $Z(0) = Z_0$ being the initial values of functions $R(t)$ and $Z(t)$ respectively. Then it can be seen that the volume $V(t) := \pi R^2(t)Z(t)$ of $D(t)$ remains constant and maintains its cylindrical form. Indeed, the points at the top of the cylinder (see Figure 4.1) move all with the same speed downwards. Those at the bottom have the downwards velocity equal to zero and those at the cylinder surface have the same radial velocity.

We now easily see that we can associate a Hamiltonian ϕ^{rz} to a point (r, z) by

$$\phi^{rz}(r, z) = \pi r^2 z,$$

so

$$\frac{\partial \phi^{rz}}{\partial\left(\frac{r^2}{2}\right)} = 2\pi z, \quad \frac{\partial \phi^{rz}}{\partial z} = 2\pi\left(\frac{r^2}{2}\right). \tag{4.3}$$

Consider a cylinder, as shown in Figure 4.1, with radius $r(t)$ and height $z(t)$. We can write the equations of motion for the point $(r(t), z(t))^T$ as follows

$$\begin{cases} \frac{d}{dt}\left(\frac{r^2}{2}\right) &= -2\pi\left(\frac{r^2}{2}\right) \\ \frac{d}{dt}z &= 2\pi z \end{cases} \tag{4.4}$$

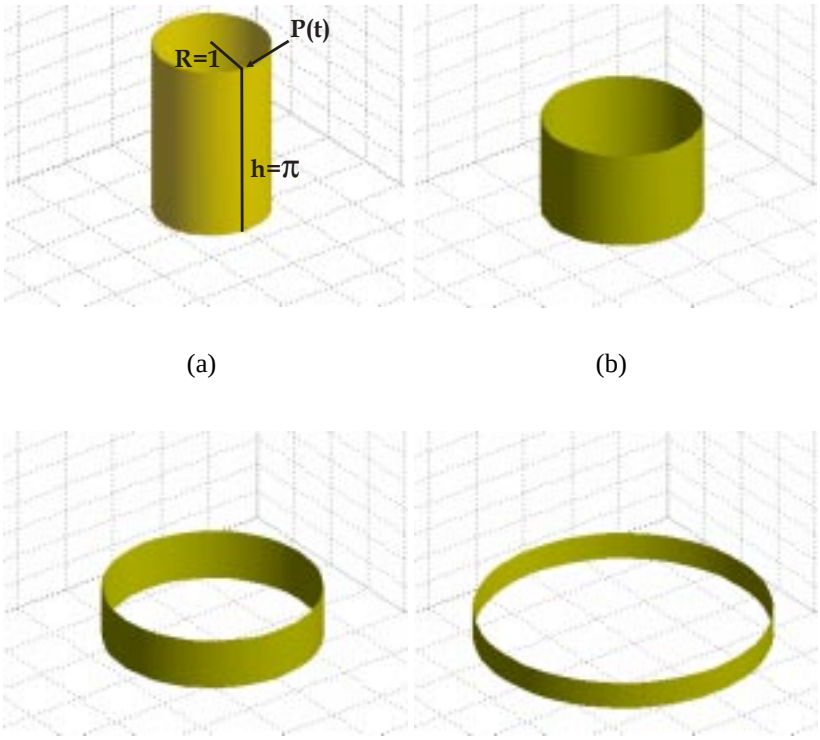


Figure 4.1: Cylinder evolution in time.

Let us first consider the non-conservative system of ordinary differential equations. We obtain for r and z

$$\begin{cases} \dfrac{dr}{dt} &= -\pi r, \\ \dfrac{dz}{dt} &= 2\pi z. \end{cases} \tag{4.5}$$

Since this system is linear, the midpoint rule (3.3) immediately gives

$$\begin{cases} r^{k+1} &= \left(\dfrac{1-\Delta t\,\pi/2}{1+\Delta t\,\pi/2}\right) r^k, \\ z^{k+1} &= \left(\dfrac{1+\Delta t\,\pi}{1-\Delta t\,\pi}\right) z^k. \end{cases} \tag{4.6}$$

Hence, the numerically computed volumes at step k and $(k+1)$, $V^{rz\,k}$ and $V^{rz\,k+1}$ say, are related

as follows

$$V^{rzk+1} = \pi (r^{k+1})^2 z^{k+1} = \left(\frac{1 - \Delta t\, \pi/2}{1 + \Delta t\, \pi/2}\right)^2 \left(\frac{1 + \Delta t\, \pi}{1 - \Delta t\, \pi}\right) V^{rzk}.$$

Since the factor on the right-hand side is of order $1 + O(\Delta t^2)$, we conclude that we will not have volume conservation.

If we now use the scheme (3.5) instead, we have

$$\begin{cases} (r^{k+1})^2 &= \left(\dfrac{1 - \Delta t\pi}{1 + \Delta t\pi}\right)(r^k)^2, \\ \\ z^{k+1} &= \left(\dfrac{1 + \Delta t\pi}{1 - \Delta t\pi}\right) z^k. \end{cases} \tag{4.7}$$

It is trivial to see that we have volume conservation now.

We have performed a numerical simulation of $P(t)$, a point at the top edge of the cylinder (see Figure 4.1a), 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 4.2 we have plotted the volume as a function of t for N the number of correction steps being equal to $0,\ 1,\ 4$ and 8. For $N = 8$ we appear to have full accuracy (up to round-off error).

Example 2. The next example deals with a non-linear problem. Consider a cylindrically symmetric three dimensional velocity field

$$\begin{cases} u_r &= -\dfrac{1}{8} r^4 \cos z, \\ \\ u_z &= \dfrac{1}{2} r^2 \sin z \end{cases} \tag{4.8}$$

Since (2.7) is satisfied, the velocity field above is divergence free. Rewriting r, z in terms of x, y (see (2.8)) gives

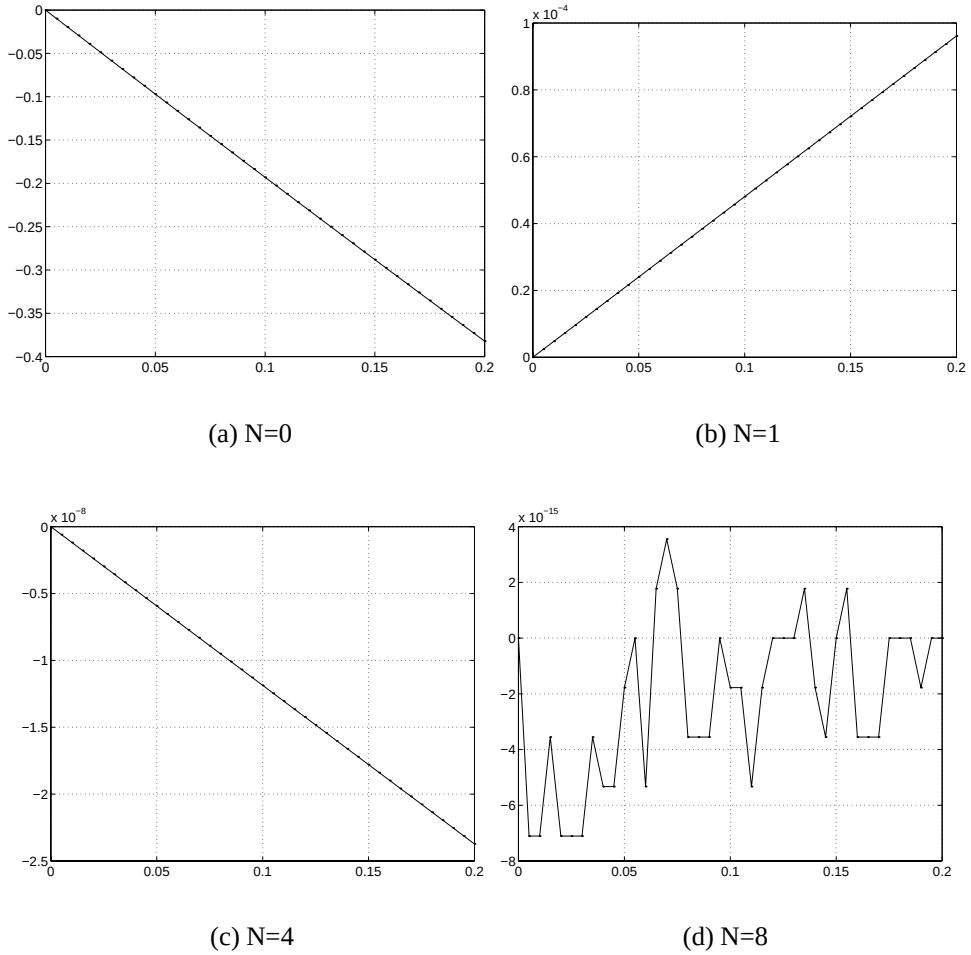
$$\begin{cases} u_x &= -\dfrac{1}{2} x^2 \cos y, \\ \\ u_y &= x \sin y. \end{cases} \tag{4.9}$$

This system is a Hamiltonian system. Indeed, one can easily find the expression for the Hamiltonian itself:

$$\phi^{xy}(x, y) = \frac{1}{2} x^2 \sin y.$$

Consider a cylinder as shown in Figure 4.3. The radius of the cylinder is 1 and the height is π. The initial position of the cylinder's upper and lower planes correspond to $z = \pi$ and $z = 0$ respectively. Clearly, the relative positions 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:

$$V^{rz}(t) := \frac{\pi}{3} \int_0^{\pi} (r^2(z) + r(z) + 1)\, dz,$$



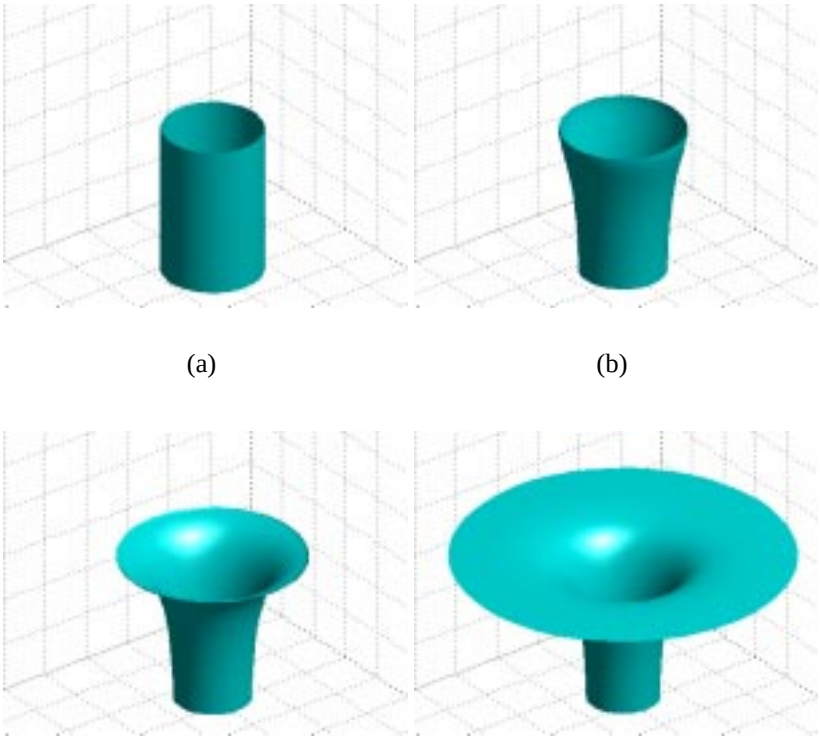
(a) N=0 (b) N=1

(c) N=4 (d) N=8

Figure 4.2: Volume graphs for different number of mid-point correction steps (Example 1).

where $r(z)$ is a function describing the geometry of an axisymmetrical body at time t.

As was illustrated in the first example, conservation of volume depends on a number of correction steps, used in the mid-point rule. Since we have a more complicated surface that requires numerical integration we have another parameter, M say, that indicates the number of intervals used in an equispaced trapezoidal rule. We like to point out that this M is not relevant for our method as such (and indeed a higher order quadrature formula would do a much better job). In this example an additional parameter arises from integration formula above. Figure 4.4 illustrates how accuracy is depending on M.



(a) (b)

(c) (d)

Figure 4.3: Frustum evolution in time.

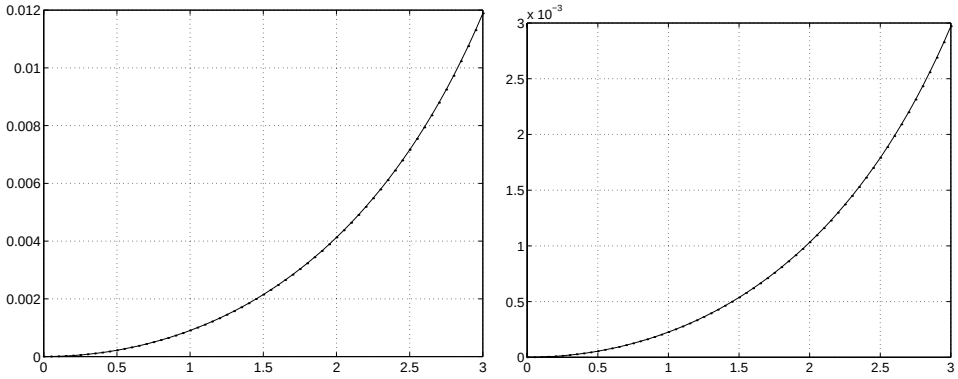
5 Computing the Flow of a Viscous Blob

In this section we shall consider a real life problem, where conservation of mass is fairly important for the actual utilisation. Consider a mould as in Figure 5.1. Here glass is pressed to a final shape by a moving part, the plunger (for more details see [2]). The problem is to describe the glass flow and, more in particular, to find out the position of the free boundary Γ_f (see Figure 5.1). Since the problem is axisymmetric we use cylindrical coordinates r and z to turn it into a two dimensional problem. We can model this problem by the Stokes creeping flow equation. For the velocity $\mathbf{v}$ and pressure p of the glass, we have

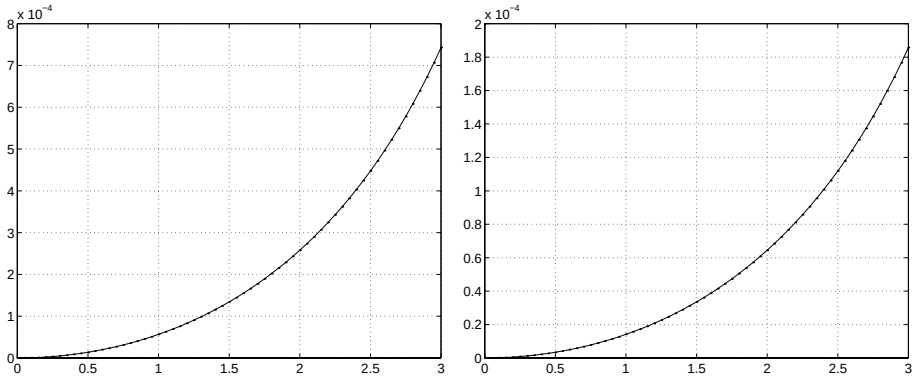
$$\begin{aligned} \nabla^2 \mathbf{v} - \nabla p &= 0 \\ \nabla \cdot \mathbf{v} &= 0. \end{aligned} \tag{5.1}$$

This equation has to be provided with boundary conditions (among which the kinematic condition, involved by the plunger motion).

At any particular time point we can thus compute the velocity field. Note that this is not available in closed form now. We may solve (5.1) by some sufficiently accurate solver (finite volume or (mixed) finite element methods). The resulting problem is then to solve $\mathbf{x}$, the position of the



(a) M=32 (b) M=64



(c) M=128 (d) M=256

Figure 4.4: Volume graphs for different number of integration intervals (Example 2).

glass, from the ordinary differential equation

$$\frac{d\mathbf{x}}{dt} = \mathbf{v}(\mathbf{x}), \tag{5.2}$$

where $\mathbf{x} \in \Omega_t$, the glass domain (see Figure 5.1). The fact that a time stepping method needs to incorporate the constraint $\mathbf{x} \in \Omega_{t_{k+1}}$, requires an additional procedure. Indeed , by discretising the free boundary we may consider a Lagrangian approach for the mesh point.

Consider first in more detail the deformation of the free boundary during a time step. Applying (3.3) to a point $\mathbf{x}_i^k$ at the boundary Γ_f^k (i.e. the boundary Γ_f at time t_k) with corresponding velocities $\mathbf{v}_i^k$ we see that some of the points $\mathbf{x}_i^{k+1}$ don't belong to the physical domain as defined by the mould and the plunger. Let us denote the latter by $\Theta_{t_{k+1}}$. This configuration is changed explicitly by moving the plunger at each time iteration. We now simply clip displacement outside this $\Theta_{t_{n+1}}$, see Figure 5.2. So the new position of $\mathbf{x}_i^{k+1}$, $\hat{\mathbf{x}}_i^{k+1}$ say is defined now by intersection of

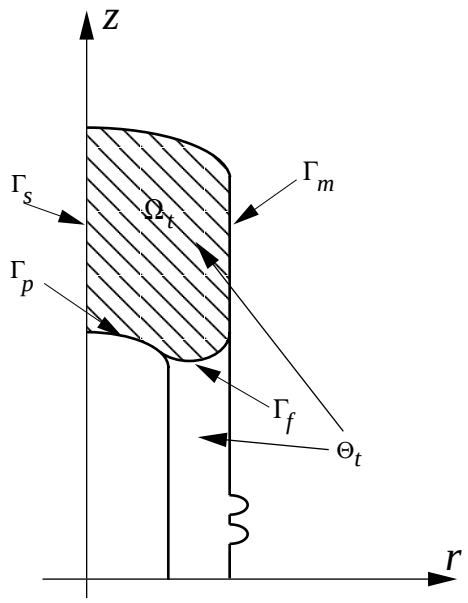


Figure 5.1: Problem domain.

$\mathbf{x}_i^{k+1}$ and $\Theta_{t_{n+1}}$:

$$\hat{\mathbf{x}}_i^{k+1} = \mathbf{x}_i^k + \alpha_i(\mathbf{x}_i^{k+1} - \mathbf{x}_i^k), \quad \alpha_i \in (0, 1],$$

where α_i is chosen such that $\Omega_{t_{k+1}} \in \Theta_{t_{k+1}}$. We call this algorithm the "clip" algorithm.

It is outside the scope of this paper to show how the midpoint rule actually blends in nicely with the clip algorithm (implying only higher order losses). In Figure 5.3a we show the dramatic effect of an explicit method for the mass conservation. In Figure 5.3b we give the result for the midpoint rule. In both cases we have taken $\Delta t = 0.005$.

References

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

[2] K.Laevsky, R.M.M.Mattheij, *Mathematical Modeling of Some Glass Problems,* In Complex Flows in Industrial Processes, Ed. A.Fasano. Birkhäuser 1999, 191-214.

[3] E.Hairer, S.P. Nørsett, G.Wanner, *Solving Ordinary Differential Equations I*, New York: Springer-Verlag, 1987.

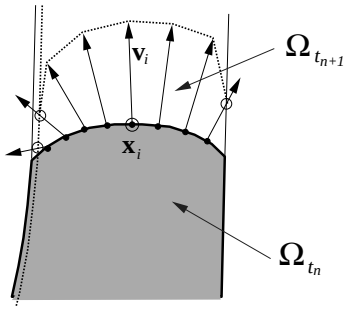
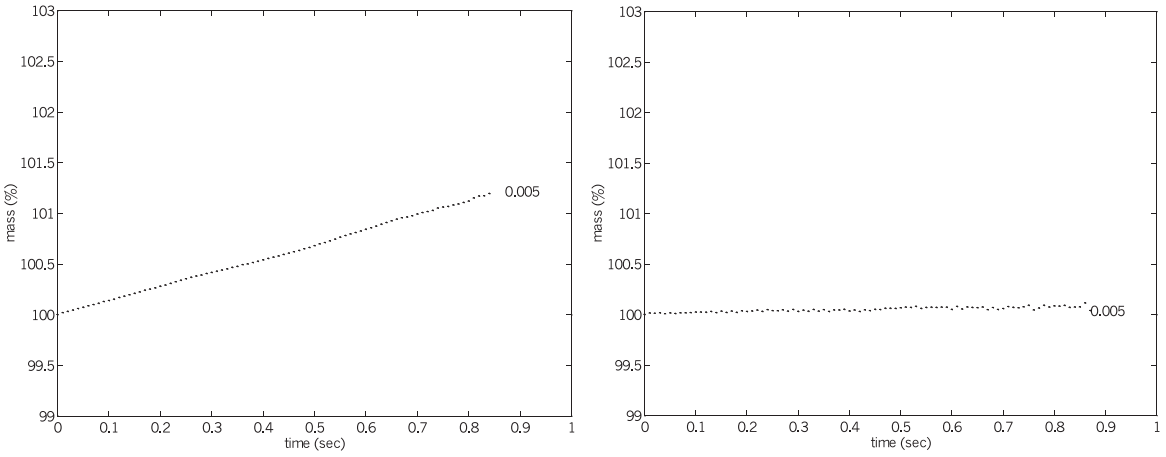


Figure 5.2: Clip algorithm.



(a) Explicit scheme

(b) Midpoint rule

Figure 5.3: Volume graphs for the different integration schemes.