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by

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Preface

This technical report is a chapter from the term project report "Numerisk analyse av tidsintegratorer for koplet analyse av strømning rundt fleksible konstruksjoner" (in Norwegian) by the two authors, submitted June, 2000. It is the only chapter written in English, but it is believed that it can be read independently of the other parts of the term project. I have taken the liberty of removing two references to other parts of the term project. Apart from this, the present report is identical to Chapter 4 of the term project. It has been some demand for this work from the international research community, this is the reason why it has been issued as a technical report of the Department of Mathematical Sciences.

Trondheim, November 2001, Brynjulf Owren.

1 Introduction

The purpose of this section is to investigate the order of various time integrators on dynamic meshes. The section consists of four parts.

The first two parts are closely related to the material in [3], in which a numerical investigation of the time accuracy for a family of time integrators, based on the second order backward difference formula (BDF-2), is performed. The time integrators are applied to CFD-problems on dynamic meshes, with special attention to the diffusive flux. In the first part we formalize the order analysis for this family of time integrators.

The second part gives an alternative approach to the process of developing a method which numerically retains second order, using techniques with certain similarities to [3]. The main idea is to consider the diffusive flux as a perturbation of a simplified problem with convection only.

In the third part we develop a generalized multistep method, that includes the family of time integrators in [3] as well as linear multistep methods in general. We perform an order analysis of this generalized scheme, and find the conditions the scheme must satisfy to be of a certain order.

We end the section by verifying numerically the theoretical results obtained in the three previous parts, solving the unsteady heat equation using finite differences on a domain with one moving boundary. We also implement the finite element method in one case, to see if this will affect the numerical order estimations.

2 Generalized BDF-2

In computational fluid dynamics (CFD), BDF schemes are often used as time integrators. For any equation of the form $\frac{dy}{dt} = f(t, y)$, BDF-2 is given by

$$\frac{3}{2}y^{n+1} - 2y^n + \frac{1}{2}y^{n-1} = \Delta t f(t^{n+1}, y^{n+1}), \tag{1}$$

where $y^{n+i} = y(t^{n+i})$.

We begin with a quick résumé of some of the material discussed in [3]. Here the use of this scheme for CFD on dynamic meshes has been investigated. The equation to be solved is of the form

$$\frac{d}{dt}[A(x(t))W(t)] = f_d[x(t), W(t)] - f_c[x(t), \dot{x}(t), W(t)], \tag{2}$$

where $x(t)$ is the position of the grid points at time t, $\dot{x}(t)$ is the velocity of the grid points, and $W(t)$ represents the solution, that is, the fluid state vector. The terms $f_d[x(t), W(t)]$ and $f_c[x(t), \dot{x}(t), W(t)]$ are the diffusive and convective components of the flux respectively.

Integrating (2) between t^n and t^{n+1} yields

$$A^{n+1}W^{n+1} = A^n W^n + \int_{t^n}^{t^{n+1}} f_d[x(t), W(t)]dt - \int_{t^n}^{t^{n+1}} f_c[x(t), \dot{x}(t), W(t)]dt. \tag{3}$$

The evaluation of these integrals raise the question of where to evaluate the convective and diffusive fluxes; on the mesh configuration at t^n, on that at t^{n+1} or on any other linear combination of possible mesh configurations.

With this background the authors of [3] propose a generalized scheme, built on the regular BDF-2, that allows f_d and f_c to be evaluated on different linear combinations of mesh configurations. We call this *the generalized BDF-2*. It is given by

$$\begin{aligned}&\frac{3}{2}A^{n+1}W^{n+1} - 2A^n W^n + \frac{1}{2}A^{n-1}W^{n-1} \\ &= \Delta t \sum_{t=0}^{T} \{w_t^d f_d(x^{n_t^d}, W^{n+1}) - w_t^c f_c(x^{n_t^c}, \dot{x}^{n_t^c}, W^{n+1})\},\end{aligned} \tag{4}$$

where w_t^d and w_t^c are real coefficients satisfying $\sum_{t=0}^{T} w_t^d = \sum_{t=0}^{T} w_t^c = 1$. The terms $x^{n_t^d}$, $x^{n_t^c}$ and $\dot{x}^{n_t^c}$ are different linear combinations of the mesh configurations $(x^{n-l}, ..., x^n, ..., x^{n+m})$

and their velocities $(\dot{x}^{n-l}, ..., \dot{x}^{n}, ..., \dot{x}^{n+m})$, respectively. The constants l and m can be chosen arbitrarily.

Before moving further, we make two comments regarding time integrators designed for CFD-problems.

Traditionally most of the attention has been payed to the treatment of the convective flux, while the diffusive flux for simplistic reasons has been evaluated on the mesh configuration at time t^n. For high Reynolds numbers, that is when the convection is the dominating part of the flux, this might be a good approximation. But for low Reynolds numbers, the diffusive flux must be treated with care.

Secondly, it is desireable that these time integrators predict exactly the state of a uniform flow. This condition can be formulated as a Geometric Conservation Law (GCL). It can be shown that this only affects the convective part of the integrator, that is, the choice of the coefficients w_t^c, the mesh configurations $x^{n_t^c}$ and their velocities $\dot{x}^{n_t^c}$. More material regarding this subject can be found in [4]. In this paper, as well as in [3], the issue is how to handle the diffusive flux.

In [3], the scheme in (4) is used to examine numerically how the evaluation of the diffusive flux at different mesh configurations affects the time accuracy of the time integrator. The aim is to find a scheme for the diffusive flux that retains as much as possible the second order time accuracy that caracterizes the BDF-2 on fixed grids. However, the paper gives no formal order analysis for the proposed scheme.

Now, we will formalize the order analysis for the generalized BDF-2 in (4). In general, this is not a second order scheme. The order will depend on the choice of the parameters w_t and the linear combinations of mesh configurations x^{n_t} . To find the conditions that ensure that this scheme is of second order, we consider the regular BDF-2, where f is evaluated in the next time step (x^{n+1}, W^{n+1}). We know that BDF-2 is of second order, so if we substitute the exact solution $\tilde{W}$ into (1) we get

$$\begin{aligned}
&\frac{3}{2}A^{n+1}\tilde{W}^{n+1} - 2A^{n}\tilde{W}^{n} + \frac{1}{2}A^{n-1}\tilde{W}^{n-1} = \\
&\Delta t f_d(x^{n+1}, \tilde{W}^{n+1}) - \Delta t f_c(x^{n+1}, \dot{x}^{n+1}, \tilde{W}^{n+1}) + O(\Delta t^3).
\end{aligned} \tag{5}$$

This yields the following second order conditions for the right hand side of (4)

$$\sum_{t=0}^{T} w_t^d f_d(x^{n_t^d}, \tilde{W}^{n+1}) = f_d(x^{n+1}, \tilde{W}^{n+1}) + O(\Delta t^2), \tag{6}$$

$$\sum_{t=0}^{T} w_t^c f_c(x^{n_t^c}, \dot{x}^{n_t^c}, \tilde{W}^{n+1}) = f_c(x^{n+1}, \dot{x}^{n+1}, \tilde{W}^{n+1}) + O(\Delta t^2). \tag{7}$$

This will ensure that the resulting scheme is of order two. Note that w_t and x^{n_t} can be chosen independently for the diffusive and convective fluxes, as long as (6) and (7) is satisfied. Also note that (7) does not ensure that the resulting scheme satisfies the GCL. Using this result we proceed with the order analysis of the diffusive part of (4), by looking at the following method from [3]

$$\frac{3}{2}A^{n+1}W^{n+1} - 2A^nW^n + \frac{1}{2}A^{n-1}W^{n-1} = \Delta t f_d(\alpha x^n + (1-\alpha)x^{n+1}, W^{n+1})$$
$$- \frac{1}{2}\Delta t f_c(\frac{1}{2}x^{n-1} + \frac{1}{2}x^n, W^{n+1}) + \frac{3}{2}\Delta t f_c(\frac{1}{2}x^n + \frac{1}{2}x^{n+1}, W^{n+1}). \tag{8}$$

This scheme can be found from (4) by the following choices

$$\begin{aligned}
&T = 1,\ l = 0,\ m = 1,\\
&w_0^d = 0,\ w_1^d = 1,\ w_0^c = \tfrac{1}{2},\ w_1^c = -\tfrac{3}{2},\\
&x^{n_1^d} = \alpha x^n + (1-\alpha)x^{n+1},\\
&x^{n_0^c} = \tfrac{1}{2}x^{n-1} + \tfrac{1}{2}x^n,\ x^{n_1^c} = \tfrac{1}{2}x^n + \tfrac{1}{2}x^{n+1}.
\end{aligned} \tag{9}$$

The scheme for the convective flux is chosen because it can be shown to be of second order due to the restrictions in (7), and because it satisfies the GCL.

For the specific problem where the function f_d is the diffusive term of the Navier Stokes equations, it is claimed in [3] that using this scheme with $\alpha = \frac{1}{2}$, at least numerically, retains the second order time accuracy of the original BDF-2 scheme. Our aim is to formalize the order restrictions for this scheme, for an arbitrary α. Using the conditions given by (6), we know that to obtain second order time accuracy the following must be true.

$$f_d(\alpha x^n + (1-\alpha)x^{n+1}, W^{n+1}) = f_d(x^{n+1}, W^{n+1}) + O(\Delta t^2).$$

We find the Taylor expansion of $f_d(\alpha x^n + (1-\alpha)x^{n+1}, W^{n+1})$ about $t = t^{n+1}$, and use the fact that

$$x(t^n) = x(t^{n+1} - \Delta t) = x(t^{n+1}) - \Delta t\ \dot{x} + O(\Delta t^2).$$

This yields the following

$$\begin{aligned}
f_d(\alpha x^n + (1-\alpha)x^{n+1}, W^{n+1}) &= f_d(x^{n+1} - \alpha\Delta t\ \dot{x} + O(\Delta t^2), W^{n+1})\\
&= f_d(x^{n+1}, W^{n+1}) - \alpha\Delta t\ \dot{x} f_{d_x}(x^{n+1}, W^{n+1}) + O(\Delta t^2).
\end{aligned} \tag{10}$$

This shows that this method is of order $p = 2$ only if $\alpha = 0$, which recovers the regular BDF-2 scheme. The scheme proposed above with $\alpha = \frac{1}{2}$ is thus only of order $p = 1$.

In [3], the choice $\alpha = \frac{1}{2}$, is based on the following reasoning. It is claimed that evaluating the following integral

$$\int_{t^n}^{t^{n+1}} f_d[x(t), W(t^{n+1})]dt, \tag{11}$$

with second order accuracy will retain, as much as possible on moving grids, the second order of the method in total. We have shown, that the restrictions in (6) and (7) are necessary to ensure second order. Hence it is clear that an accurate approximation of this integral is not sufficient to ensure order two for the total method.

3 Developing time integration schemes using perturbation theory

The aim of this section is to show an alternative method for finding a method which numerically retains second order for the problem in (2). In this approach we take advantage of the situation when the problem equation can be considered as a perturbation of a simplified problem equation.

This approach has some similarities with what has been done in [3], because it involves the evaluation of the integral in (11). We show that an accurate evaluation of this integral indeed may give a method that numerically reveals second order. However, this is only true under the assumption that the total flux is dominated by convection, and that the diffusive term and the time step used are comparable in magnitude.

In many CFD problems, the convective flux is the dominating part of the total flux. We can then consider the contribution from the diffusive fluxes as a perturbation of the problem equation in (2) with convection only.

To simplify the notation, we let $Z = AW$ be the solution of (3), and use the fact that A and W always are evaluated at the same time. We define F_c and F_d,

$$\begin{aligned} f_c(x, \dot{x}, W) &= f_c(x, \dot{x}, A^{-1}Z) = F_c(x, \dot{x}, Z), \\ f_d(x, W) &= f_d(x, A^{-1}Z) = F_d(x, Z). \end{aligned}$$

Using this notation, we can rewrite (2) as follows

$$\dot{Z} = -F_c(x, \dot{x}, Z) + F_d(x, Z), \ t > t^n \text{ and } Z(t^n) = Z^n. \tag{12}$$

If $|F_d| \ll |F_c|$, one can consider (12) as a perturbation of the equation

$$\dot{Y} = -F_c(x, \dot{x}, Y), \ t > t^n \text{ and } Y(t^n) = Z^n. \tag{13}$$

Let us assume that we solve (13), using a second order scheme. We can now use the following two theorems which consider how small perturbations in a differential equation affect the solution. Using our notation, the first theorem (Theorem 14.5 in [1]) is as follows.

Theorem (Alexejev-Gröbner). Suppose that $\frac{\partial F_c}{\partial Y}$ exists and is continuous. Then the solutions Y and Z of (13) and the "perturbed" equation (12) are connected by

$$Z^{n+1} = Y^{n+1} + \int_{t^n}^{t^{n+1}} \frac{\partial Y(t^{n+1}, Z(s))}{\partial Z} F_d(s) ds. \tag{14}$$

Here $F_d(s) = F_d(x(s), Z(s))$ and $Y(t^{n+1}, Z(s))$ is the solution of (13) at time t^{n+1} with initial value $Y(s) = Z(s)$. The term $\frac{\partial Y}{\partial Z}$ is the derivative of $Y(t^{n+1}, Z(s))$ with respect to the initial condition $Z(s)$.

We want to simplify the integral in (14) by using the second theorem (Theorem 14.3 in [1]).

Theorem. Suppose that $\frac{\partial F_c}{\partial Y}$ exists and is continuous. Then the solutions $Y(t^{n+1}, Z(s))$ are differentiable with respect to the initial condition $Z(s)$, and the derivative is given by

$$\frac{\partial Y(t^{n+1}, Z(s))}{\partial Z} = B(t^{n+1}, s), \tag{15}$$

where B is the solution of the so-called "variational equation"

$$\begin{aligned} \frac{\partial B(t^{n+1}, s)}{\partial t} &= -\frac{\partial F_c(t^{n+1}, Y(t^{n+1}, Z(s)))}{\partial Y})B(t^{n+1}, s), \\ B(s, s) &= I. \end{aligned} \tag{16}$$

For abbreviation we have let $F_c(t^{n+1}, Y(t^{n+1}, Z(s))) = F_c(x^{n+1}, \dot{x}^{n+1}, Y(t^{n+1}, Z(s)))$. Now we can find the two leading terms of the Taylor expansion of B about $t = s$. This yields

$$\begin{aligned} B(t^{n+1}, s) &= B(s, s) + (t^{n+1} - s)\frac{dB(s, s)}{dt} + O(\Delta t^2) \\ &= I - (t^{n+1} - s)\frac{\partial F_c(s, Z(s))}{\partial Y} + O(\Delta t^2). \end{aligned} \tag{17}$$

Here we have used the following

$$\frac{dB(t^{n+1}, s)}{dt} = \frac{\partial B(t^{n+1}, s)}{\partial t} \quad \text{and} \quad Y(s, Y(s)) = Z(s). \tag{18}$$

Using (15) - (17), we can rewrite (14).

$$\begin{aligned} Z^{n+1} &= Y^{n+1} + \int_{t^n}^{t^{n+1}} B(t^{n+1}, s)F_d(s)ds \\ &= Y^{n+1} + \int_{t^n}^{t^{n+1}} F_d(s)ds - \int_{t^n}^{t^{n+1}} (t^{n+1} - s)\frac{\partial F_c(s, Z(s))}{\partial Y}F_d(s)ds + O(\Delta t^3). \end{aligned} \tag{19}$$

We compute Y^{n+1} using the second order scheme, $Y^{n+1} = \Gamma_n(F_c, \Delta t, Y^0, \dots, Y^n)$. Hence, the scheme introduces a local error of $O(\Delta t^3)$.

From (19) we see that to maintain order two of the total method, the two integrals must be evaluated with second order accuracy.

We have already assumed that $|F_d| \ll |F_c|$. Now, we assume that for the time steps used in practice, $|F_d| \sim O(\Delta t)$. Then, when integrating over an interval of length Δt, the last integral will be of an order of magnitude of $O(\Delta t^3)$, and this justifies considering only the first integral.

Using this last assumption, we rewrite (19) as follows

$$Z^{n+1} = Y^{n+1} + \int_{t^n}^{t^{n+1}} F_d(s)ds + O(\Delta t^3). \tag{20}$$

This situation can be compared to that in [3]. The convective "part", Y, of the equation has been approximated with second order accuracy. We are searching for an approximation to the integral that will retain second order accuracy for the method in total. Using interpolatory quadrature, we have the following result (e.g. from [2]).

Interpolatory Quadrature - The Midpoint Rule. If $F_d(x(t), Z(t)) \in C^2[t^n, t^{n+1}]$, then

$$\int_{t^n}^{t^{n+1}} F_d(x(s), Z(s))ds = \Delta t F_d(x^{n+1/2}, Z^{n+1/2}) + O(\Delta t^3), \tag{21}$$

when integrating over one timestep Δt.

By this result, we obtain second order accuracy, by evaluating the integral using the midpoint $(x^{n+1/2}, Z^{n+1/2})$. With this approximation, our method retains second order numerically and can be written

$$Z^{n+1} = \Gamma_n(F_c, \Delta t, Y^0, \dots, Y^n) + \Delta t F_d(x^{n+1/2}, Z^{n+1/2}). \tag{22}$$

We want to emphasize that what we have done here, is an alternative way of finding a method which numerically retains second order for the CFD problem where one wants to treat the diffusive and convective fluxes in different manners. The approach has some similarites with what has been done in [3], but does not explain the findings in this paper.

4 Generalized multistep method

In this part we generalize the scheme (4) and find the conditions for obtaining a certain order. We do not consider separation of f, because we want to isolate the issue of where to evaluate the diffusive flux.

Our generalized multistep method is given by

$$\sum_{j=0}^{s} \alpha_j A^{n+j} W^{n+j} = \Delta t \sum_{j=0}^{s} \sum_{t=0}^{T} w_{jt} f(\sum_{r=-l}^{m} \gamma_{tr} x^{n+j+r}, W^{n+j}). \tag{23}$$

Note that this method allows evaluation of f at different linear combinations of x, but not at linear combinations of W. The left hand side of this scheme is no longer that of BDF-2, but can be chosen freely.

We have let the constants γ_{tr} be independent of the index j. This is because we want a numerical scheme where the function f needs to be evaluated only once for every W_i. If we let the constants γ vary with j, we cannot reuse the already computed values of f when moving to the next time step.

This general scheme contains many well known time integration schemes, in addition to the generalized BDF-2 from the previous subsection. If we let $T = 0$, $l = m = 0$ and $\gamma_{0,0} = 1$ we get the general scheme for linear multistep methods which includes all the BDF schemes, the Euler methods and the trapezoidal rule.

Before looking further into the order restrictions, just a few words about stability and convergence of multistep methods. From chapter three we know that a multistep method of order

$p > 2$ can not be A-stable. However, for a multistep method to converge it must be of order $p \geq 1$ and obey the root condition. This fact must be kept in mind in the development of numerical schemes.

Consistency of (23) is ensured by the following requirements

$$\sum_{j=0}^{s} \alpha_j = 0, \tag{24}$$

$$\sum_{r=-l}^{m} \gamma_{tr} = 1, \ \forall \ t. \tag{25}$$

Taylor expansion of (23) about (x^n, W^n) yields

$$\begin{aligned}
&\sum_{j=0}^{s} \alpha_j \sum_{k=0}^{\infty} \frac{(j\Delta t)^k}{k!} \frac{d^k}{dt^k}(A^n W^n) \\
&-\Delta t \sum_{j=0}^{s} \sum_{t=0}^{T} w_{jt} \sum_{k=0}^{\infty} \frac{1}{k!} \left(\sum_{i=1}^{\infty} \frac{\Delta t^i}{i!} \left[\sum_{r=-l}^{m} \gamma_{tr} (j+r)^i \frac{d^i x}{dt^i} \frac{\partial}{\partial x} + j^i \frac{d^i W}{dt^i} \frac{\partial}{\partial W} \right] \right)^k f(x^n, W^n) \\
&= O(\Delta t^{p+1}),
\end{aligned} \tag{26}$$

where p is the order of the method. Up to order 3 we get the following restrictions on the method

$$\sum_{j=0}^{s} \alpha_j = 0, \tag{27}$$

$$\sum_{j=0}^{s} \left[j\alpha_j - \sum_{t=0}^{T} w_{jt} \right] = 0, \tag{28}$$

$$\sum_{j=0}^{s} \left[\alpha_j \frac{j^2}{2} - \sum_{t=0}^{T} w_{jt} \sum_{r=-l}^{m} \gamma_{tr} (j+r) \right] = 0, \tag{29}$$

$$\sum_{j=0}^{s} \left[\alpha_j \frac{j^2}{2} - \sum_{t=0}^{T} w_{jt} j \right] = 0, \tag{30}$$

$$\sum_{j=0}^{s} \left[\alpha_j \frac{j^3}{3} - \sum_{t=0}^{T} w_{jt} \sum_{r=-l}^{m} \gamma_{tr} (j+r)^2 \right] = 0, \tag{31}$$

$$\sum_{j=0}^{s} \left[\alpha_j \frac{j^3}{3} - \sum_{t=0}^{T} w_{jt} j^2 \right] = 0, \tag{32}$$

$$\sum_{j=0}^{s} \left[\alpha_j \frac{j^3}{3} - \sum_{t=0}^{T} w_{jt} \left(\sum_{r=-l}^{m} \gamma_{tr} (j+r) \right)^2 \right] = 0, \tag{33}$$

$$\sum_{j=0}^{s} \left[\alpha_j \frac{j^3}{3} - \sum_{t=0}^{T} w_{jt} \sum_{r=-l}^{m} \gamma_{tr} (j+r) j \right] = 0. \tag{34}$$

For methods of order less than 3, the restrictions (27)-(28) ensure order 1, while (27)-(30) ensure order 2. If we return to the general scheme for linear multistep methods by letting $T = 0$, $l = m = 0$ and $\gamma_{0,0} = 1$, the above restrictions simplify to

$$\sum_{j=0}^{s} \alpha_j = 0, \tag{35}$$

$$\sum_{j=0}^{s} (j\alpha_j - w_{j,0}) = 0, \tag{36}$$

$$\sum_{j=0}^{s} (\frac{j^2}{2}\alpha_j - jw_{j,0}) = 0, \tag{37}$$

$$\sum_{j=0}^{s} (\frac{j^3}{3}\alpha_j - j^2 w_{j,0}) = 0, \tag{38}$$

which correspond to the well known order conditions for linear multistep methods.

If we further restrict the general scheme by letting $w_{0,0} = 0, w_{1,0} = 0, \ldots, w_{s-1,0} = 0$ and $w_{s,0} \neq 0$ we get the s-order BDF schemes. For $s = 3$, the restrictions above give the following equations to be solved

$$\alpha_0 + \alpha_1 + \alpha_2 + \alpha_3 = 0, \tag{39}$$

$$\alpha_1 + 2\alpha_2 + 3\alpha_3 - w_{3,0} = 0, \tag{40}$$

$$\frac{1}{2}\alpha_1 + 2\alpha_2 + \frac{9}{2}\alpha_3 - 3w_{3,0} = 0, \tag{41}$$

$$\frac{1}{3}\alpha_1 + \frac{8}{3}\alpha_2 + 9\alpha_3 - 9w_{3,0} = 0. \tag{42}$$

Solving these equations gives us the BDF-3 scheme

$$A^{n+3}W^{n+3} - \frac{18}{11}A^{n+2}W^{n+2} + \frac{9}{11}A^{n+1}W^{n+1} - \frac{2}{11}A^n W^n = \frac{6}{11}\Delta t f(x^{n+3}, W^{n+3}). \tag{43}$$

We end this section by finding a new third order method based on the generalized scheme in (23), using the following parameters

$$\begin{aligned} &s = 2,\ T = 1,\ l = 1,\ m = 1, \\ &\gamma_{0,-1} = 1/2,\ \gamma_{0,1} = 1/2,\ \gamma_{1,-1} = -\frac{1}{2},\ \gamma_{1,0} = 2\ \gamma_{1,1} = -\frac{1}{2}. \end{aligned} \tag{44}$$

We thus have 8 degrees of freedom in our scheme and 8 conditions to obtain a method of order $p = 3$. Solving this system of linear equations yields a scheme with the following constants

$$\begin{aligned} &\alpha_0 = -\frac{1}{5},\ \alpha_1 = -\frac{4}{5},\ \alpha_2 = 1, \\ &w_{0,0} = -\frac{1}{5},\ w_{0,1} = \frac{1}{5},\ w_{1,0} = \frac{4}{5},\ w_{1,1} = 0,\ w_{2,0} = 0,\ w_{2,1} = \frac{2}{5}. \end{aligned} \tag{45}$$

This scheme obeys the root condition, since the two zeros of the characteristic polynomial are, $z_- = -\frac{1}{5}$ and $z_+ = 1$. In the next section we implement this scheme, and compare it to BDF-3.

5 Numerical estimation of order

Here we estimate numerically the order of several time integrators mentioned in the previous parts, all of which fit into the general scheme in (23).

We have considered the model problem

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \quad t > 0, \ x \in \Omega(t) = (x_0(t), 1), \tag{46}$$

where

$$u(x, 0) = 4x(1 - x), \tag{47}$$
$$u(x_0(t), t) = u(1, t) = 0, \tag{48}$$

and $x_0(t)$ is the position of the left boundary. We have looked at the case where the left boundary moves with constant speed, $K > 0$, with $x_0(0) = 0$, and the case where the movement of the left boundary is described by the function $x_0(t) = 0.5\sin(6\pi t)$. Note that in this model problem we consider heat transfer by diffusion only, that is $f_c \equiv 0$.

As spatial distretization we have used both finite differences and finite elements. Both cases lead to a system of ODE's which can be written

$$\dot{v}_i(t) \ = \ f(x(t), v(t)), \tag{49}$$

where $v_i(t)$ is the numerical solution at the i'th node. To solve this system we use the following methods:

1. Generalized BDF-2

Here we have implemented the generalized BDF-2 in (8), which in this case is given by

$$\frac{3}{2}A^{n+1}W^{n+1} - 2A^nW^n + \frac{1}{2}A^{n-1}W^{n-1} = \Delta t f(\alpha x^n + (1-\alpha)x^{n+1}, W^{n+1}), \tag{50}$$

where $f = f_d$, since $f_c \equiv 0$.

The experiments are done evaluating f at three different mesh configurations $x(t)$

(i) The current position $x(t^n)$: $\alpha = 1$.

(ii) The midpoint $\frac{1}{2}x(t^n) + \frac{1}{2}x(t^{n+1})$: $\alpha = \frac{1}{2}$.

(iii) The next position $x(t^{n+1})$: $\alpha = 0$.

Our aim is to confirm the results from the order analysis in the previous section. That is, to see which mesh configuration gives the best order numerically. These methods are implemented using both finite differences and finite elements, to see if the different discretizations give the same results.

2. Third order methods

The third order moving grid method (MGM-3) from (44)-(45) written out yields

$$\begin{aligned}
&v^{n+2} - \frac{4}{5}v^{n+1} - \frac{1}{5}v^{n} = \\
&\Delta t \left[-\frac{1}{5}f(\frac{1}{2}x^{n-1} + \frac{1}{2}x^{n+1}, v^{n}) + \frac{1}{5}f(-\frac{1}{2}x^{n-1} + 2x^{n} - \frac{1}{2}x^{n+1}, v^{n}) \right. \\
&\left. +\frac{4}{5}f(\frac{1}{2}x^{n} + \frac{1}{2}x^{n+2}, v^{n+1}) + \frac{2}{5}f(-\frac{1}{2}x^{n+1} + 2x^{n+2} - \frac{1}{2}x^{n+3}, v^{n+2}) \right]. \qquad (51)
\end{aligned}$$

We implement this method to confirm that the third order conditions developed in (27)-(34), in fact gives a third order method. We also compare it to BDF-3 (43). Both methods are implemented using finite differences.

The exact solution of our problem is unknown because of the moving boundary. Instead we approximate the exact solution by solving the same system (with the same spatial discretization), but with a much smaller time step. We call this the reference solution.

In all the numerical experiments in this section we have used the following parameters

- $\Delta t_1 = 5 \cdot 10^{-4}$, $\Delta t_2 = 1 \cdot 10^{-3}$, $\Delta t_3 = 5 \cdot 10^{-3}$ and $\Delta t_4 = 1 \cdot 10^{-2}$
- Time step for reference solution: $\Delta t_{ref} = \frac{1}{10}\Delta t_1 = 5 \cdot 10^{-5}$
- Position of the moving boundary:
  1. $x_0(t) = Kt$, $K = 1.3$
  2. $x_0(t) = 0.5\sin(6\pi t)$
- Initial grid spacing: $h_0 = 1/10$

For an s-step method, we need the initial values $y^0, \ldots, y^{s-1}$. For the reference solution, these were approximated using Euler forward. To be able to compare the solutions using different time steps, the solutions were set to equal the reference solution up to time $t = (s-1)\Delta t_4$. This explains why the plots show no error compared to the reference solution for the first few time steps.

The error at time step n is given by

$$\|e^n_{\Delta t}\|^2 = \sum_{i=1}^{n} (V_i^n - v_i^n)^2, \qquad (52)$$

where V_i^n is the reference solution. The order p is estimated using the formula (53).

$$p \approx \frac{\ln\left[\frac{\|e_{\Delta t_2}\|}{\|e_{\Delta t_1}\|}\right]}{\ln\left[\frac{\Delta t_2}{\Delta t_1}\right]} \qquad (53)$$

Note that we have estimated the order using the results from the two smallest timesteps, Δt_1 and Δt_2.

5.1 Semidiscretization by finite differences

In the finite difference approach, the domain $[x_0(t), 1]$ is discretized as shown in fig. 1, keeping the distance $h(t)$ uniform over the entire interval.

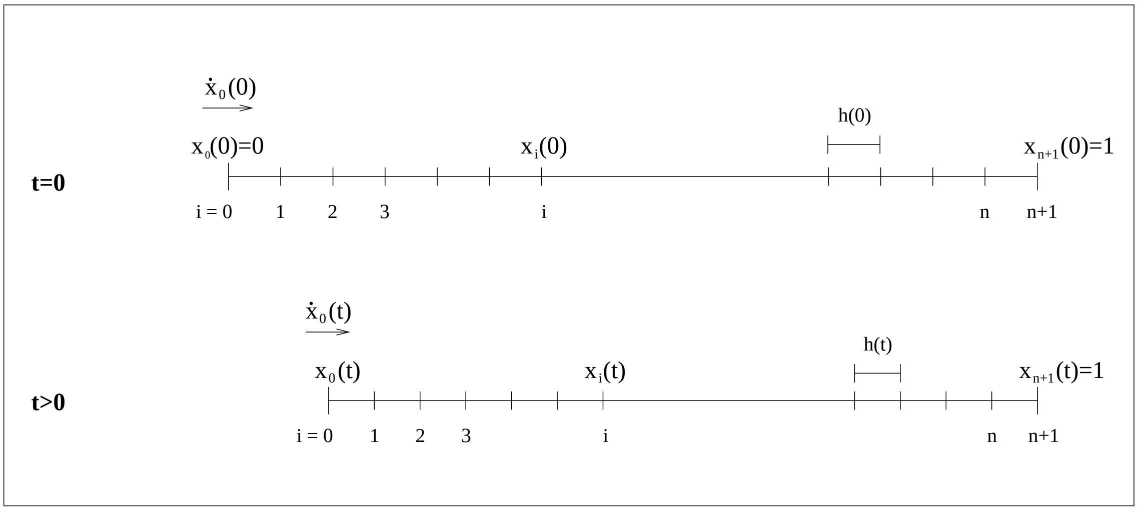

Figure 1: The grid with one boundary moving at speed $\dot{x}_0(t)$.

This means that the position of the nodes is a function of time

$$x_i = x_i(t),\ i = 0, \ldots, n+1.$$

Let

$$v_i(t) = u(x_i(t), t),\ i = 0, \ldots, n+1.$$

By differentiating $v_i(t)$ with respect to time, and using the problem equation (46), we get

$$\begin{aligned} \frac{d}{dt} v_i(t) &= \frac{\partial}{\partial x} u(x_i(t), t) \frac{d}{dt} x_i(t) + \frac{\partial}{\partial t} u(x_i(t), t), \\ &\Updownarrow \\ \dot{v}_i(t) &= u_x(x_i(t), t)\dot{x}_i(t) + u_{xx}(x_i(t), t). \end{aligned} \tag{54}$$

When $x_0(t)$ is given, it can be shown that

$$x_i(t) = \frac{i}{n+1} + x_0(t)(1 - \frac{i}{n+1}),\ i = 0, \ldots, n+1, \tag{55}$$

$$\dot{x}_i(t) = (1 - \frac{i}{n+1})\dot{x}_0(t),\ i = 0, \ldots, n+1, \tag{56}$$

$$h(t) = \frac{1 - x_0(t)}{n+1}. \tag{57}$$

We semidiscretize equation (54), using central differences

$$\begin{aligned} u_x(x_i(t),t) &= \frac{1}{2h(t)}(v_{i+1}(t) - v_{i-1}(t)) + O(h^2), \\ u_{xx}(x_i(t),t) &= \frac{1}{h(t)^2}(v_{i+1}(t) - 2v_i(t) + v_{i-1}(t)) + O(h^2). \end{aligned}$$

This gives us the equation

$$\dot{v}_i(t) = \frac{\dot{x}_i(t)}{2h(t)}(v_{i+1}(t) - v_{i-1}(t)) + \frac{1}{h(t)^2}(v_{i+1}(t) - 2v_i(t) + v_{i-1}(t)) + O(h^2), \quad (58)$$

which can be written

$$\dot{v}_i(t) = f(x(t), v(t)). \quad (59)$$

5.1.1 Numerical results for the generalized BDF-2 using finite differences

The numerical solutions and errors for the regular BDF-2, as compared to the reference solution, are shown in figures 2 and 3. The numerical order estimates for the three methods based on the scheme in (50) are shown in figures 4 and 5, and table 1.

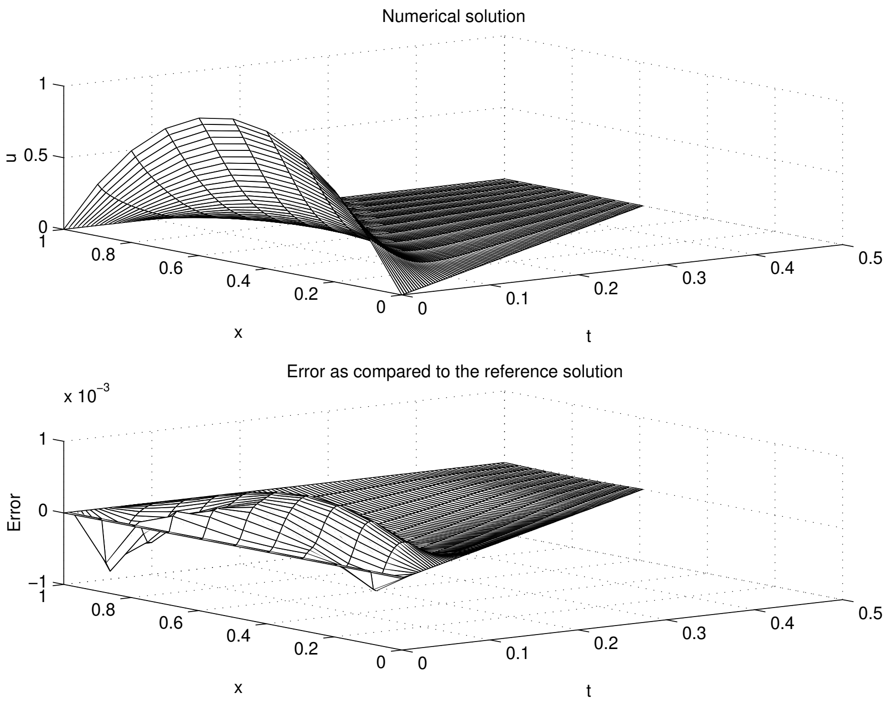

Figure 2: Numerical solution and error for the regular BDF-2 using finite differences and $x_0(t) = Kt$.

It is clear from our experiments that the regular BDF-2 gives the best results both when it comes to order and error. We also see that the midpoint approximation is of the same order

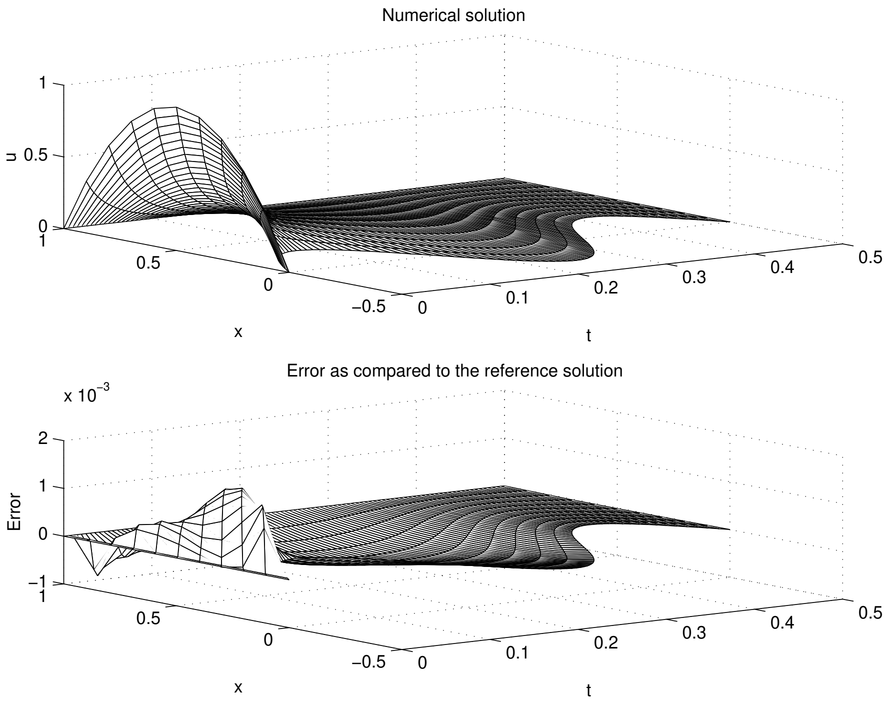

Figure 3: Numerical solution and error for the regular BDF-2 using finite differences and $x_0(t) = 0.5\sin(6\pi t)$.

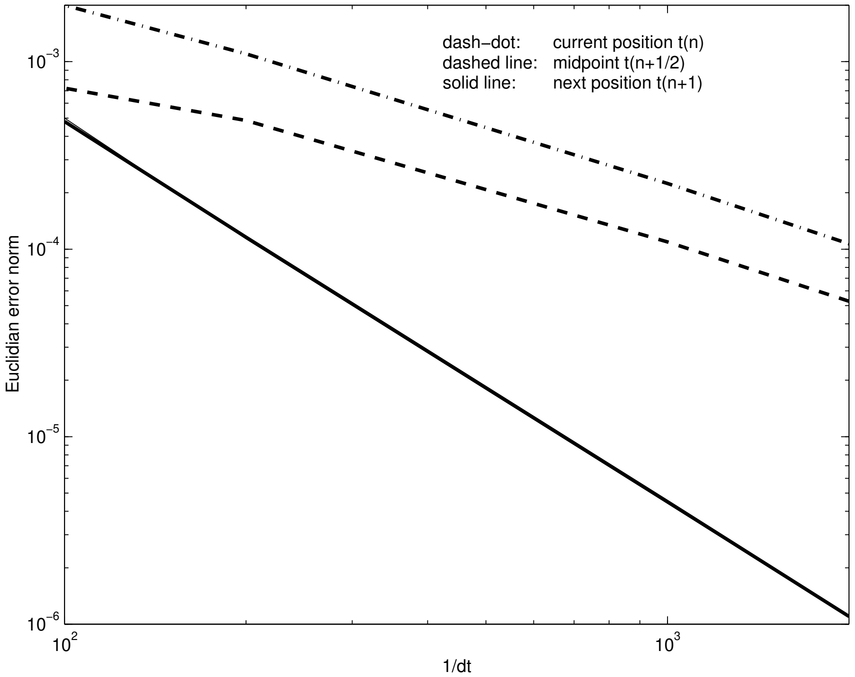

Figure 4: Numerical error versus $1/\Delta t$ for the generalized BDF-2 using finite differences and $x_0(t) = Kt$.

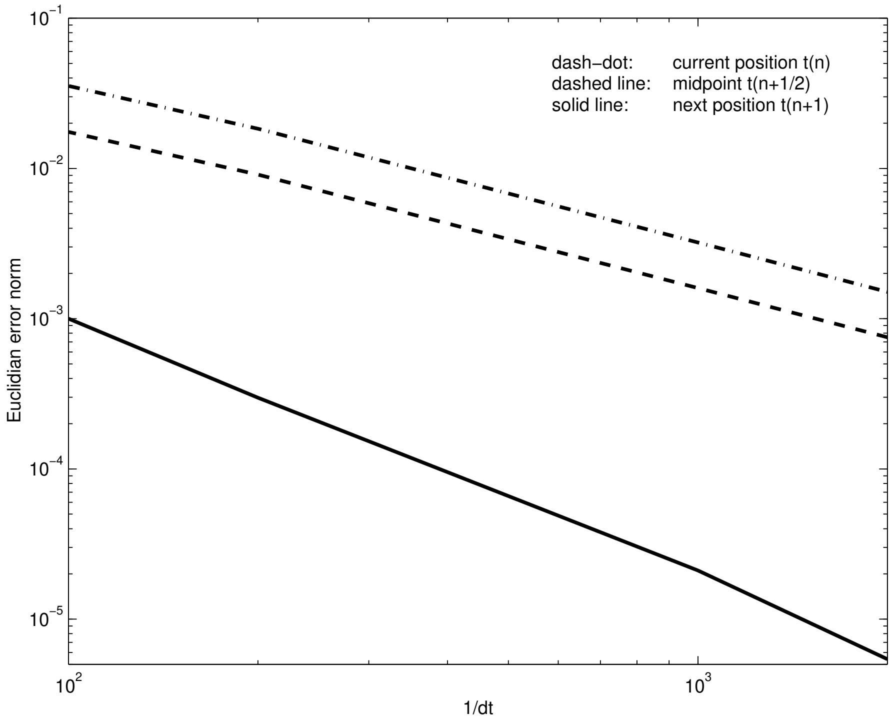

Figure 5: Numerical error versus $1/\Delta t$ for the generalized BDF-2 using finite differences and $x_0(t) = 0.5\sin(6\pi t)$.

Position of $x_0(t)$	Order of (i)	Order of (ii)	Order of (iii)
Kt	1.07	1.05	2.02
$0.5\sin(6\pi t)$	1.09	1.09	1.96

Table 1: Order of the generalized BDF-2 using finite differences.

as method (i), but gives a smaller error. The numerical order estimates confirm the result from the order analysis, namely that only the regular BDF-2 can obtain second order time accuracy.

5.1.2 Numerical results for the third order methods using finite differences

Position of $x_0(t)$	BDF-3	MGM-3
Kt	3.07	3.00
$0.5\sin(6\pi t)$	3.05	2.79

Table 2: Order of the third order methods using finite differences.

Solution and error as compared to the reference solution, for MGM-3 and BDF-3, are shown in figures 6-9. Figures 10 and 11 and table 2 show the order estimates of the methods.

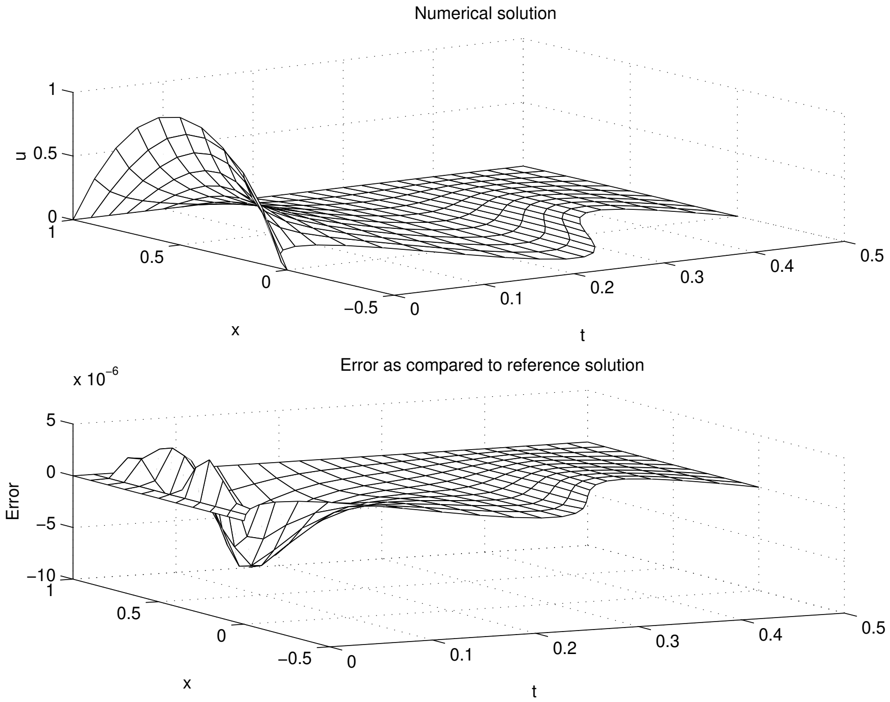

Figure 6: Numerical solution and error for MGM-3 using finite differences and $x_0(t) = 0.5\sin(6\pi t)$.

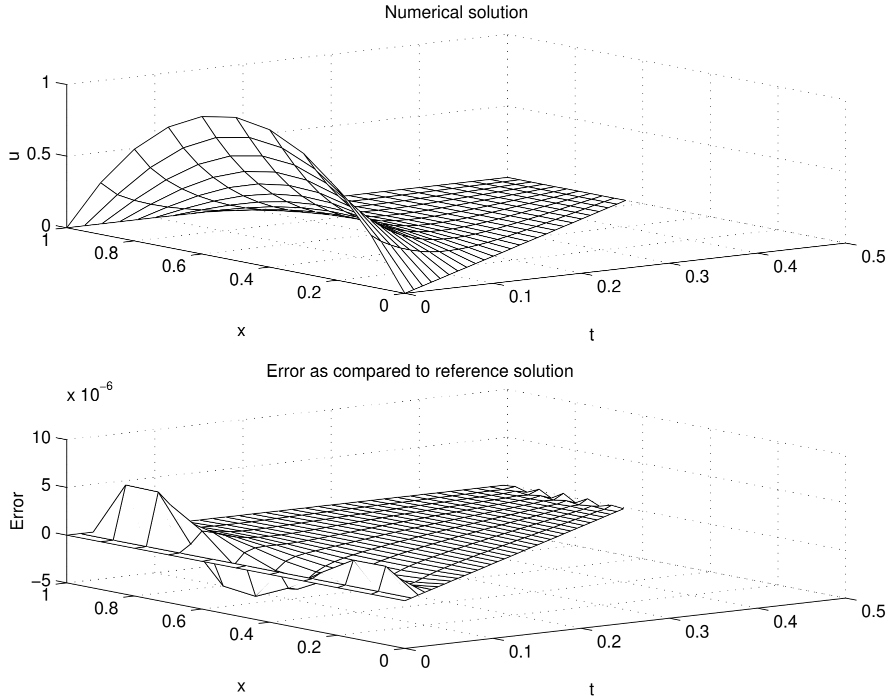

Figure 7: Numerical solution and error for MGM-3 using finite differences and $x_0(t) = Kt$.

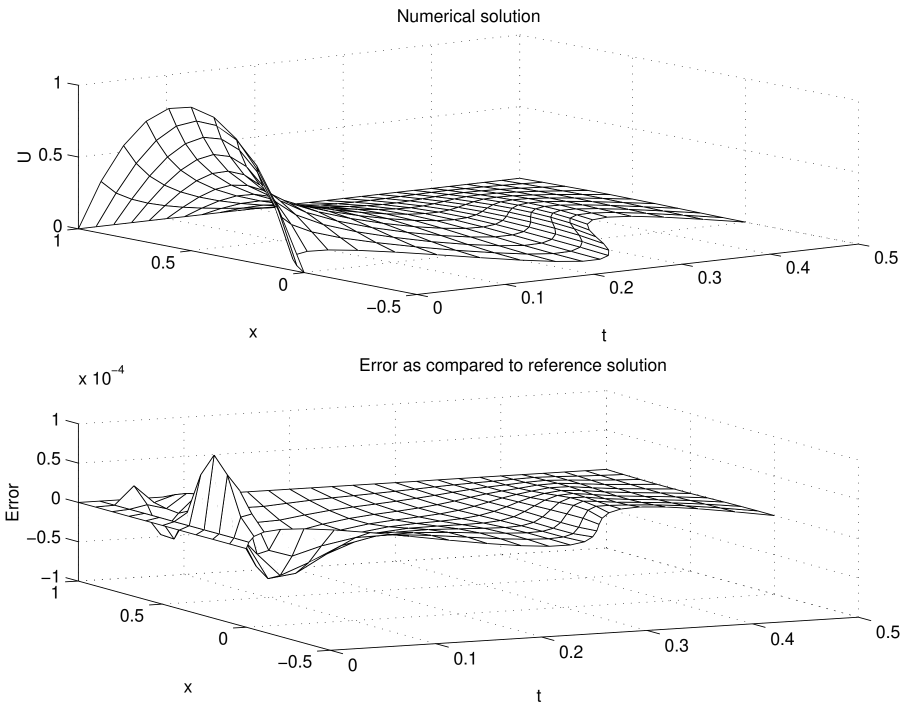

Figure 8: Numerical solution and error for BDF-3 using finite differences and $x_0(t) = 0.5\sin(6\pi t)$.

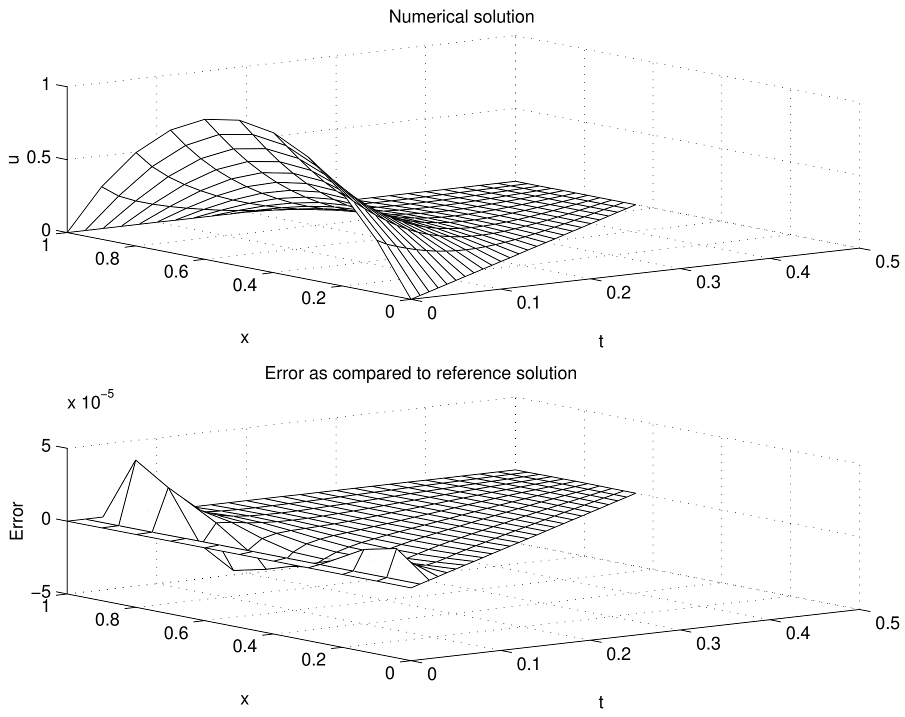

Figure 9: Numerical solution and error for BDF-3 using finite differences and $x_0(t) = Kt$.

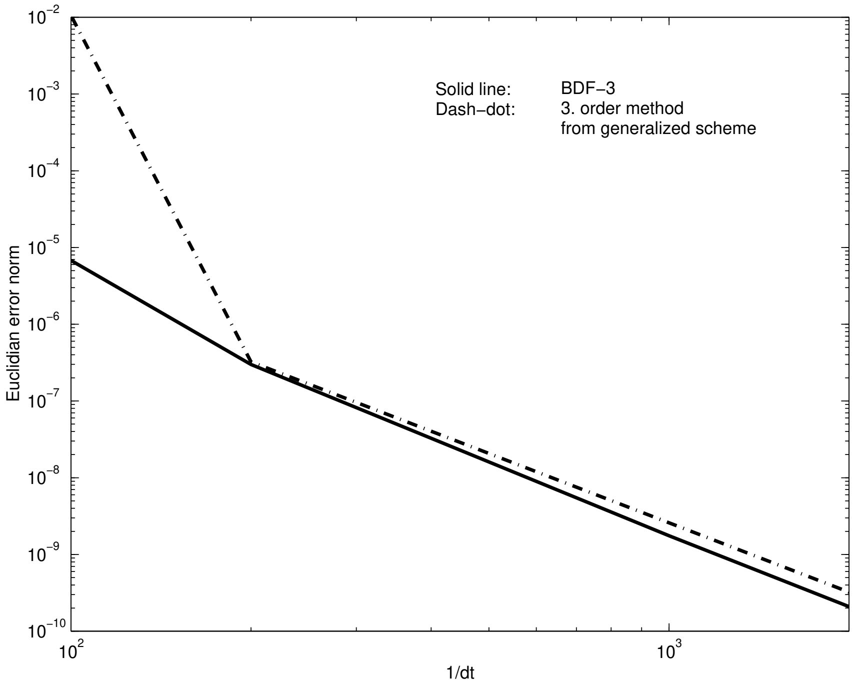

Figure 10: Numerical error versus $1/\Delta t$ for BDF-3 and MGM-3 using finite differences and $x_0(t) = 0.5\sin(6\pi t)$.

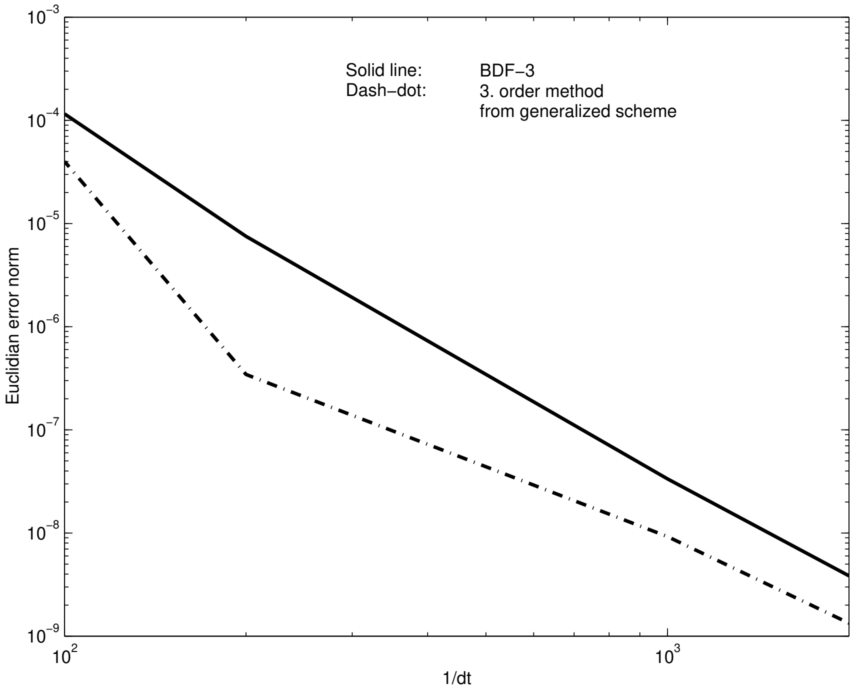

Figure 11: Numerical error versus $1/\Delta t$ for BDF-3 and MGM-3 using finite differences and $x_0(t) = Kt$.

It is clear that both methods obtain order three, even if BDF-3 seems to be slightly better than MGM-3, judging by the order estimates. When it comes to which method that has the smallest error, we see that this depends on the speed of the boundary node $x_0(t)$.

During the numerical experiments it was clear that both methods are unstable for large Δt. This is in accordance with the theory of Chapter 3, which states that no third order method can be A-stable. For our model problem with the given spatial discretization, we found that MGM-3 is stable for $\Delta t < 5 \cdot 10^{-3}$, while BDF-3 remains stable for $\Delta t < 1 \cdot 10^{-2}$.

5.2 Semidiscretization by finite elements

In this section we solve (46), with $x_0(t) = Kt$, using linear finite elements on $\Omega(t)$. This is done by a transformation onto a fixed reference configuration Ω_0. We introduce the continuous mapping

$$\begin{aligned} x : \Omega_0 \times \mathbb{R} &\rightarrow \Omega(t), \\ (\xi, t) &\rightarrow x(\xi, t), \end{aligned}$$

which maps the i'th node ξ_i, on the fixed configuration Ω_0, to its image $x(\xi_i, t)$ on the present configuration. The speed of $x(\xi_i, t)$ on $\Omega(t)$ is given by $\frac{d}{dt} x(\xi, t)|_{\xi=\xi_i}$.

Let

$$v(\xi, t) = u(x(\xi, t), t), \ t > 0, \ \xi \in [0, 1].$$

Then

$$\begin{aligned} \frac{\partial}{\partial t} u(x(\xi, t), t) &= \frac{\partial}{\partial t} v(\xi, t) = \dot{v}(\xi, t) \\ \frac{\partial}{\partial x} u(x(\xi, t), t) &= \frac{\partial}{\partial x} v(\xi, t) = \frac{\partial}{\partial \xi} v(\xi, t) \frac{d\xi}{dx} = v_\xi(\xi, t) \frac{1}{J}, \end{aligned}$$

where $J = \det \frac{dx}{d\xi} = \frac{dx}{d\xi}$ denotes the Jacobian. In our case

$$x(\xi_i, t) = \xi_i + K(1 - \xi_i)t,$$

hence

$$J = \frac{dx}{d\xi} = 1 - Kt = J(t).$$

Writing (46) in terms of ξ gives

$$\frac{\partial v}{\partial t} = \frac{1}{J(t)^2} \frac{\partial^2 v}{\partial \xi^2}, \ t > 0, \ \xi \in \Omega_0 = (0, 1), \tag{60}$$

where $v(0, t) = v(1, t) = 0$. The weak formulation of the homogenous Dirichlet problem in (60) is as follows

$$\int_0^1 (\dot{v} w + \frac{1}{J(t)^2} v_\xi w_\xi) d\xi = 0, \ \forall \ w \in X, \tag{61}$$

where

$$X = H^1_0(\Omega_0) = \{v \in H^1(\Omega_0)|\ v(0) = v(1) = 0\}. \tag{62}$$

We consider a linear finite element discretization of this problem on a triangulation $\mathcal{T}_h$ of equi-sized elements $T^k_h,\ k = 1, \dots, n+1$, where the corresponding $n+2$ nodes are given by $\xi_0 = 0, \dots, \xi_{n+1} = 1$. We search for the solution in the discrete space

$$X_h = \{v \in X|\ v|_{T^k_h} \in \mathbb{P}_1(T^k_h), k = 1, \dots, n+1\} = \text{span}\{\Phi_i(\xi),\ i = 1, \dots, n\},$$

where $\Phi_i(\xi) \in \mathbb{P}_1(\Omega_0)$ and $\Phi_i(\xi_j) = \delta_{ij}$. Hence, every $w \in X_h$ can be written

$$w(\xi) = \sum_{i=1}^{n} w_i \Phi_i(\xi). \tag{63}$$

Note that $\dim(X_h) = n$ because of the boundary conditions, and that $X_h \subset X$, which means that we use a conforming approximation. Now we can find the weak formulation of the discrete problem,

$$\int_0^1 (\dot{v}_h w + \frac{1}{J(t)^2} v_{h,\xi} w_\xi) d\xi = 0,\ \forall w \in X_h. \tag{64}$$

From (63) and (64) we get the following system

$$M_h \dot{v_h} + \frac{1}{J(t)^2} A_h v_h = 0,$$

where $M_h,\ A_h \in \mathbb{R}^{n\times n}$.

The semidiscrete system can now be written as

$$\dot{v}_h(t) \ = = -\frac{1}{J(t)^2} M_h^{-1} A_h v_h(t) = f(x(t), v_h(t)). \tag{65}$$

5.2.1 Numerical results for the generalized BDF-2 using finite elements

The equation is solved by using the generalized BDF-2 in (50) and then evaluating $J(t)$ in three different configurations as in the case of the finite difference method.

Order of (i)	Order of (ii)	Order of (iii)
1.07	1.06	2.02

Table 3: Order of the generalized BDF-2 using the finite element method and $x_0(t) = Kt$.

The results are shown in fig. 12 and table 3. These results are almost identical to those obtained from the finite difference discretization. We see that method (iii), evaluating $J(t)$ in $t = t^{n+1}$ gives an order of two, while the two other methods only reveal a first order time accuracy. For the time step interval investigated in these computations, the error is also less using method (iii) than the two other methods.

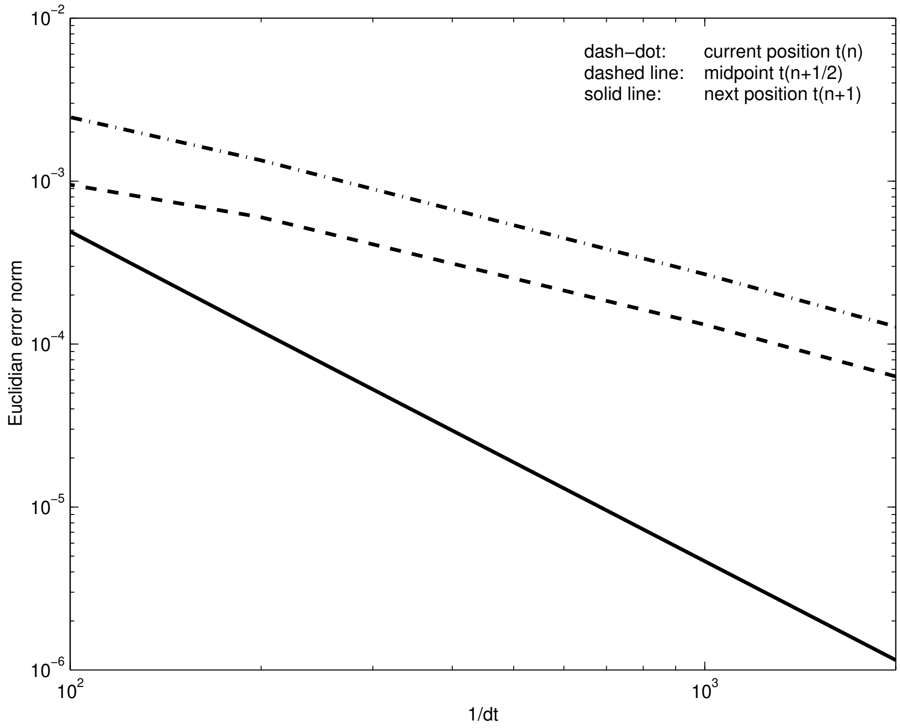

Figure 12: Numerical error versus $1/\Delta t$ for the generalized BDF-2 using the finite element method and $x_0(t) = Kt$.

6 Conclusions

In this section we have investigated various time integration methods on dynamic meshes, with the main attention to the treatment of the diffusive flux in CFD-problems.

The generalized BDF-2, given in equation (50), has been analysed, using three different choices for the mesh configuration $x(t)$ on which to evaluate $f(x(t), W(t))$. Both theoretical and numerical analysis, using both finite differences and the finite element method, gives that the only method which obtains an order 2 is the one where the mesh configuration is evaluated in time step $t = t^{n+1}$, that is, the regular BDF-2.

We have also found a scheme for a generalized multistep method and found restrictions for obtaining a certain order. We have verified these results numerically for a third order method, and compared this method to BDF-3. There were no major differences in the order estimates of the methods or in the error estimates. Both methods show signs of unstability at high time steps, but MGM-3 requires smaller time steps than BDF-3 in order to be stable. The fact that the methods are unstable for some Δt is in accordance with the theory of Chapter 3, which states that no third order method can be A-stable.

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