

DERIVATION OF THE WEAK FORM FOR A FIRST-ORDER DIFFERENTIAL EQUATION BY APPLICATION OF FRACTIONAL CALCULUS

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ABSTRACT

One important property of the finite element method is the fact that it leads to symmetric system matrices which results in advantageous numerical characteristics. The initial relation is the weak form of the underlying differential equation where a partial integration 'shifts' one order of derivative from the unknown variable to its virtual counterpart. This results in the same order of derivatives for both quantities and, since the same shape functions for each of them are used, consequently it leads to symmetric system matrices. This means in turn that only differential equations can be treated which are even-ordered. In this work we consider a first-order differential equation and apply fractional calculus to obtain a weak form which contains semi-derivatives. This serves as a starting point to deduce a respective finite-element formulation.

KEYWORDS: fractional calculus, finite element method, weak form, first-order differential equation.

1. INTRODUCTION

Even though the research field of fractional calculus is more than 300 years old it is only little known by engineers and scientists. In fact, the term 'fractional' is misleading since the order of derivatives or integrals may exhibit any real or even complex value. Nevertheless, the name 'fractional' is kept for historical reasons. One reason for the shadowy existence of fractional calculus is the missing geometrical interpretation of a fractional derivative or integral. Another reason is the lack of applications up to the 20th century. The usefulness of fractional derivatives in the framework of viscoelasticity was first realized by Nutting [7] and Gemant [5]. In the 70s Bagley and Torvik [1] started an extensive investigation of fractional calculus in viscoelasticity including appropriate parameter identifications which ensure the thermomechanical consistency of the resulting constitutive equations [2]. Since then some fundamental textbooks on fractional calculus have been published which include applications of fractional calculus to different fields in physics and engineering such as diffusion problems, control theory, chaos or image processing [8, 9, 4, 6]. In this contribution fractional calculus including a formula for fractional partial integration is used to deduce the weak form of a first-order differential equation which is the starting point for a finite-element formulation. To the best knowledge of the author such an attempt has not been made in the literature.

2. UNDERLYING DIFFERENTIAL EQUATION

In order to evaluate the different numerical approaches a simple one-dimensional first-order differential equation with constant coefficients is considered for which the analytical solution is known. In especially, the so-called barometric formula is regarded which describes the air pressure p as a function of the altitude h by

$$\frac{dp(h)}{dh} = -\frac{Mg}{RT} p(h). \quad (1)$$

In its simplest (isothermal) form the molar mass M , the acceleration of gravity g , the universal gas constant R and the temperature T are taken to be constant. Thus, the differential equation can be simplified to

$$\frac{1}{p} dp = -c dh, \quad c = \frac{Mg}{RT} = \text{const.} \quad (2)$$

A unique solution requires one boundary condition which is given by

$$p(0) = p_0 \quad (3)$$

and describes the air pressure at ground level $h = 0$.

2.1. Analytical Solution

The analytical solution is found by integration of Eq. (2)

$$\int_{p_0}^p \frac{1}{\tilde{p}} d\tilde{p} = \int_0^h -c d\tilde{h}$$

$$\ln \frac{p}{p_0} = -ch$$

$$p = p_0 \exp(-ch) \quad (4)$$

where p_0 is the boundary condition defined in Eq. (3).

2.2. Forward Difference Approximation

For our first numerical scheme we apply the finite difference method (fdm) using a forward-difference approximation of the derivative in Eq. (1) to obtain

$$\frac{p_{k+1} - p_k}{\Delta h} = -p_k c \quad (5)$$

or

$$p_{k+1} + (c\Delta h - 1)p_k = 0 \quad (6)$$

where Δh denotes the step size and the indices k and $k + 1$ denote two adjacent discretization points. In matrix notation Eqs. (3) and (6) can be written as

$$\begin{bmatrix} 1 & & & \\ c\Delta h - 1 & 1 & & \\ & c\Delta h - 1 & 1 & \\ & & \ddots & \ddots \end{bmatrix} \begin{bmatrix} p_0 \\ p_1 \\ p_2 \\ \vdots \end{bmatrix} = \begin{bmatrix} p(0) \\ 0 \\ 0 \\ \vdots \end{bmatrix}. \quad (7)$$

2.3. Backward Difference Approximation

Alternatively, we may use the fdm in conjunction with a backward-difference approximation of the derivative in Eq. (1) which leads to

$$\frac{p_{k+1} - p_k}{\Delta h} = -p_{k+1} c \quad (8)$$

or

$$(1 + c\Delta h)p_{k+1} - p_k = 0. \quad (9)$$

Together with the boundary condition Eq. (3) one obtains

$$\begin{bmatrix} 1 & & & \\ -1 & 1 + c\Delta h & & \\ & -1 & 1 + c\Delta h & \\ & & \ddots & \ddots \end{bmatrix} \begin{bmatrix} p_0 \\ p_1 \\ p_2 \\ \vdots \end{bmatrix} = \begin{bmatrix} p(0) \\ 0 \\ 0 \\ \vdots \end{bmatrix}. \quad (10)$$

2.4. Finite Element Approximation

Since we are dealing with a first-order differential equation a finite element formulation with symmetric system matrices cannot be deduced using classical calculus. However, a finite element formulation with a nonsymmetric system matrix can be deduced applying the method of weighted residuals to the underlying Differential Equation (1)

$$\int_0^\ell w \left(\frac{dp}{dh} + cp \right) dx = 0 \quad (11)$$

In Eqs. (21) and (22) n is a natural number such that

$$n - 1 < \alpha < n \quad (23)$$

holds. Since only semi derivatives and semi integrals occur, i.e. $\alpha = 1/2$, Eqs. (19) — (22) simplify to

$$\text{RL}I_{a+}^{\frac{1}{2}}q(t) = \frac{1}{\Gamma(1/2)} \int_a^t \frac{q(\tau)}{\sqrt{(t-\tau)}} d\tau \quad (24)$$

$$\text{RL}I_{b-}^{\frac{1}{2}}q(t) = \frac{1}{\Gamma(1/2)} \int_t^b \frac{q(\tau)}{\sqrt{(\tau-t)}} d\tau \quad (25)$$

$$\text{RL}D_{a+}^{\frac{1}{2}}q(t) = \frac{1}{\Gamma(1/2)} D^1 \int_a^t \frac{q(\tau)}{\sqrt{(t-\tau)}} d\tau = D^1 \left(\text{RL}I_{a+}^{\frac{1}{2}}q(t) \right) \quad (26)$$

$$\text{RL}D_{b-}^{\frac{1}{2}}q(t) = \frac{-1}{\Gamma(1/2)} D^1 \int_t^b \frac{q(\tau)}{\sqrt{(\tau-t)}} d\tau = -D^1 \left(\text{RL}I_{b-}^{\frac{1}{2}}q(t) \right). \quad (27)$$

Note that the semi derivatives can directly be calculated from the semi integrals by application of an ordinary first-order derivative. In order to obtain a symmetric system matrix from Eq. (11) we modify the first term of the integrand using the composition rule of fractional calculus

$$\int_0^\ell w D^1 p dx = \int_0^\ell w \left(\text{RL}D_{0+}^{\frac{1}{2}} \text{RL}D_{0+}^{\frac{1}{2}} p \right) dx \quad (28)$$

which holds as long as

$$\text{RL}I_{0+}^{\frac{1}{2}} \left(\text{RL}D_{0+}^{\frac{1}{2}} p \right) = p \quad (29)$$

is fulfilled, see e.g. [8]. Application of fractional partial integration Eq. (18) yields

$$\int_0^\ell w D^1 p dx = \int_0^\ell \text{RL}D_{\ell-}^{\frac{1}{2}} w \text{RL}D_{0+}^{\frac{1}{2}} p dx + \text{RL}I_{\ell-}^{\frac{1}{2}} w(\ell) \text{RL}D_{0+}^{\frac{1}{2}} p(\ell) - w(0)p(0), \quad (30)$$

where Condition (29) is used to deduce the last term of Eq. (30). A finite-element ansatz for Eq. (11) with linear shape functions for the field variable p and the weight function w as given in Eqs. (12) and (13) and making use of Eq. (30) results in

$$\underline{w}^T \left(\int_0^\ell \text{RL}D_{\ell-}^{\frac{1}{2}} \underline{H}^T \text{RL}D_{0+}^{\frac{1}{2}} \underline{H} dx + \text{RL}I_{\ell-}^{\frac{1}{2}} \underline{H}^T(\ell) \text{RL}D_{0+}^{\frac{1}{2}} \underline{H}(\ell) - \underline{H}^T(0) \underline{H}(0) + c \int_0^\ell \underline{H}^T \underline{H} dx \right) \underline{p} = 0 \quad (31)$$

For a further evaluation of Eq. (31) the right and left semi integrals of the shape functions h_1 and h_2 have to be calculated. Having in mind that fractional operators are linear, i.e.

$$I^\alpha(c_1 f_1 + c_2 f_2) = c_1 I^\alpha(f_1) + c_2 I^\alpha(f_2), \quad c_1, c_2 = \text{const.} \quad (32)$$

holds for all fractional operators $I_{a+}, I_{b-}, D_{a+}, D_{b-}$ (see e.g.[8]) it is sufficient to consider a constant and a linear function. Using Eqs. (24) and (25) we obtain

$$\text{RL}I_{0+}^{\frac{1}{2}}(1) = \frac{1}{\Gamma(1/2)} \int_0^x \frac{1}{\sqrt{x-\tau}} d\tau = \frac{-1}{\sqrt{\pi}} [2\sqrt{x-\tau}]_0^x = \frac{2}{\sqrt{\pi}} \sqrt{x} \quad (33)$$

$$\text{RL}I_{0+}^{\frac{1}{2}}(x) = \frac{1}{\Gamma(1/2)} \int_0^x \frac{\tau}{\sqrt{x-\tau}} d\tau = \frac{-1}{\sqrt{\pi}} \left[\frac{2}{3}(\tau+2x)\sqrt{x-\tau} \right]_0^x = \frac{4}{3\sqrt{\pi}} x\sqrt{x} \quad (34)$$

$$\text{RL}I_{\ell-}^{\frac{1}{2}}(1) = \frac{1}{\Gamma(1/2)} \int_x^\ell \frac{1}{\sqrt{\tau-x}} d\tau = \frac{1}{\sqrt{\pi}} [2\sqrt{\tau-x}]_x^\ell = \frac{2}{\sqrt{\pi}} \sqrt{\ell-x} \quad (35)$$

$$\text{RL}I_{\ell-}^{\frac{1}{2}}(x) = \frac{1}{\Gamma(1/2)} \int_x^\ell \frac{\tau}{\sqrt{\tau-x}} d\tau = \frac{1}{\sqrt{\pi}} \left[\frac{2}{3}(\tau+2x)\sqrt{\tau-x} \right]_x^\ell = \frac{2}{3\sqrt{\pi}} (\ell+2x)\sqrt{\ell-x}. \quad (36)$$

Therefore we have

$${}^{\text{RL}}\mathbf{I}_{0+}^{\frac{1}{2}}(h_1) = \frac{2}{\sqrt{\pi}} \left(1 - \frac{2x}{3\ell}\right) \sqrt{x} \quad (37)$$

$${}^{\text{RL}}\mathbf{I}_{0+}^{\frac{1}{2}}(h_2) = \frac{4}{3\sqrt{\pi}} \frac{x}{\ell} \sqrt{x} \quad (38)$$

$${}^{\text{RL}}\mathbf{I}_{\ell-}^{\frac{1}{2}}(h_1) = \frac{4}{3\sqrt{\pi}} \left(1 - \frac{x}{\ell}\right) \sqrt{\ell-x} \quad (39)$$

$${}^{\text{RL}}\mathbf{I}_{\ell-}^{\frac{1}{2}}(h_2) = \frac{2}{3\sqrt{\pi}} \left(1 + 2\frac{x}{\ell}\right) \sqrt{\ell-x}. \quad (40)$$

The fractional semi derivatives can be derived from Eqs. (37) – (40) using relationships (26) and (27) which yields

$${}^{\text{RL}}\mathbf{D}_{0+}^{\frac{1}{2}}(h_1) = \mathbf{D}^1 \left({}^{\text{RL}}\mathbf{I}_{0+}^{\frac{1}{2}}(h_1) \right) = \frac{1}{\sqrt{\pi}} \left(\frac{1}{\sqrt{x}} - 2\frac{\sqrt{x}}{\ell} \right) \quad (41)$$

$${}^{\text{RL}}\mathbf{D}_{0+}^{\frac{1}{2}}(h_2) = \mathbf{D}^1 \left({}^{\text{RL}}\mathbf{I}_{0+}^{\frac{1}{2}}(h_2) \right) = \frac{2}{\sqrt{\pi}} \frac{\sqrt{x}}{\ell} \quad (42)$$

$${}^{\text{RL}}\mathbf{D}_{\ell-}^{\frac{1}{2}}(h_1) = \mathbf{D}^1 \left({}^{\text{RL}}\mathbf{I}_{\ell-}^{\frac{1}{2}}(h_1) \right) = \frac{2}{\sqrt{\pi}} \frac{\sqrt{\ell-x}}{\ell} \quad (43)$$

$${}^{\text{RL}}\mathbf{D}_{\ell-}^{\frac{1}{2}}(h_2) = \mathbf{D}^1 \left({}^{\text{RL}}\mathbf{I}_{\ell-}^{\frac{1}{2}}(h_2) \right) = \frac{1}{\sqrt{\pi}} \left(\frac{1}{\sqrt{\ell-x}} - 2\frac{\sqrt{\ell-x}}{\ell} \right). \quad (44)$$

From Eqs. (39) – (42) we see that the expression ${}^{\text{RL}}\mathbf{I}_{\ell-}^{\frac{1}{2}}\underline{H}^T(\ell){}^{\text{RL}}\mathbf{D}_{0+}^{\frac{1}{2}}\underline{H}(\ell)$ in (31) vanishes. Making use of Eqs. (41) – (44) the first term in Eq. (31) can be evaluated by performing the necessary integrations. Thus, we finally get

$$\int_0^{\ell} {}^{\text{RL}}\mathbf{D}_{\ell-}^{\frac{1}{2}}\underline{H}^T {}^{\text{RL}}\mathbf{D}_{0+}^{\frac{1}{2}}\underline{H} dx = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}. \quad (45)$$

Since the third term in (31) is

$$\underline{H}^T(0)\underline{H}(0) = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \quad (46)$$

the resulting equation for one finite element reads

$$\left(\frac{1}{2} \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix} + \frac{c\ell}{6} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \right) \begin{bmatrix} p_1 \\ p_2 \end{bmatrix} = \frac{1}{6} \begin{bmatrix} -3+2c\ell & 3+c\ell \\ -3+c\ell & 3+2c\ell \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \end{bmatrix} = \underline{0} \quad (47)$$

which is exactly the same result obtained without the use of fractional calculus, see Eq. (16). However, symmetry of the system's matrix is not achieved in the above derivation due to the occurrence of left and right fractional derivatives of the shape functions.

4. COMPARISON OF THE APPROACHES

A comparison between the different schemes is realized using the values given in Table 1, where the data from the International Standard Atmosphere is applied and the temperature is taken to be constant.

Table 1 – Values used within the barometric formula.

molar mass M	gravitational constant g	universal gas constant R	absolute temperature T
28.95 g/mol	9.807 m/s ²	8.314 J/(mol K)	288.15 K

Thus, the constant c is given by

$$c = \frac{Mg}{RT} = 1.185 \cdot 10^{-4} \frac{1}{\text{m}}. \quad (48)$$

The Dirichlet boundary condition which is needed to obtain a unique solution is given by the air pressure at sea level

$$p(0) = 1.0135 \text{ bar} \quad (49)$$

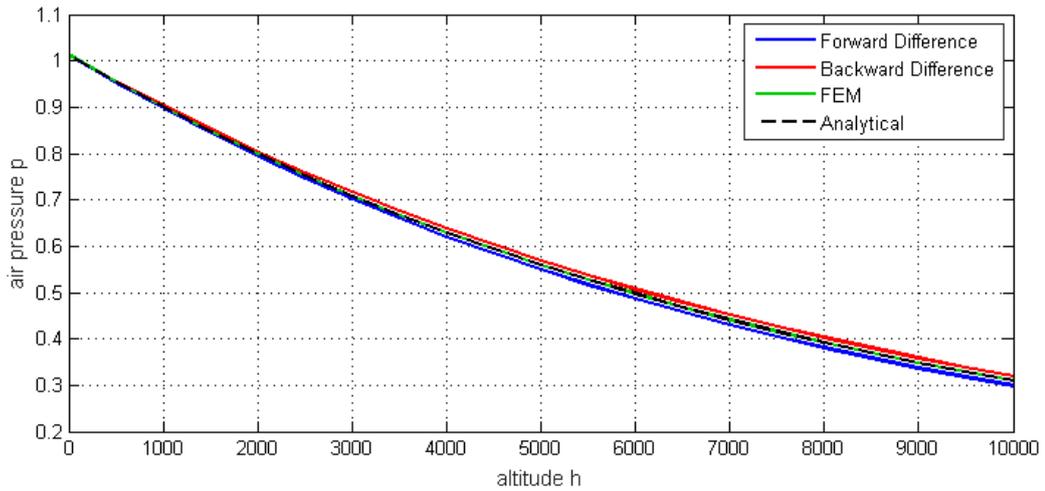


Figure 1 – Comparison between the different numerical schemes and the analytical solution.

and is also taken from the International Standard Atmosphere.

The air pressure is calculated for a height $h \in [0\text{m}, 10000\text{m}]$ using a spacing Δh of 500m where the result of all schemes is displayed along with the analytical solution, see Figure 1. All schemes converge as expected as the spacing Δh is reduced. However, as can be seen from Figure 2 the finite element method with a non-symmetric system matrix by far performs best.

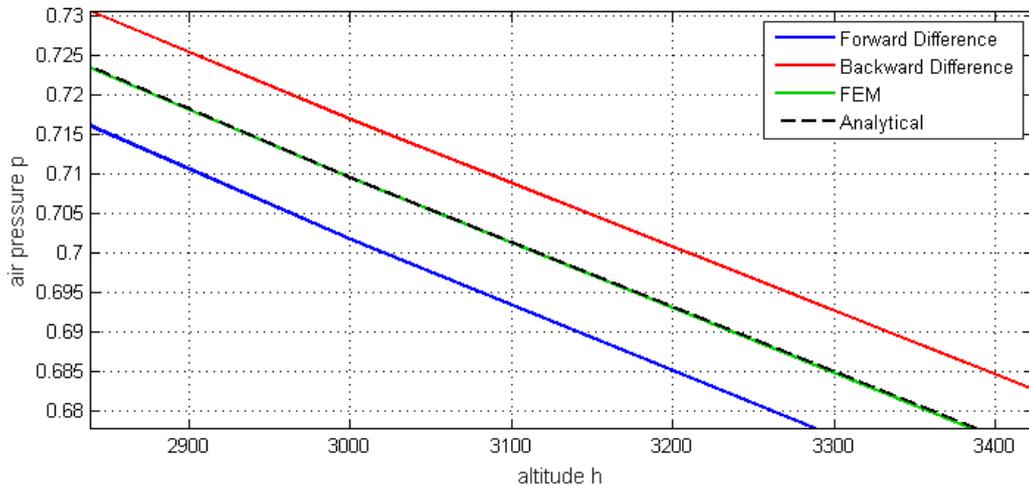


Figure 2 – Image enlargement of the results.

5. CONCLUSION

The main goal of this research work was the derivation of the weak form of a first-order differential equation by application of fractional calculus. Since the weak form requires the same order of derivative for both quantities the field variable and its virtual counterpart partial fractional integration of order $1/2$ has to be applied. The resulting weak form served as the basic equation for a finite-element formulation which should result in symmetric system matrices. However, since forward and backward fractional derivatives/integrals occur, the symmetry could not be achieved. Nevertheless, compared to finite-difference approximations the resulting scheme performs much better. A closer look at the system matrix shows that it coincides with the system matrix obtained without application of fractional partial integration. If this is generally the case also for higher-order shape functions still has to be examined. As an alternative approach Petrov-Galerin method could be used instead of Bubnov-Galerin method

where the weight functions are directly derived from the requirements of symmetry. In addition, the use of Caputo-type fractional derivatives instead of the classical Riemann-Liouville ones may lead to better results.

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