

# Comparison of current methods for polymer analysis by boundary elements

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## Abstract

In this paper, quasi-static analyses of polymers, based on the boundary element method, are reviewed and implemented. Linear viscoelasticity, for which the correspondence principle applies, is assumed. Thus, one of the adopted BEM approaches solves the problem in the Laplace transform domain and relies on numerical inversion for the determination of the time-dependent response. The second solves directly in the time domain using fundamental solutions specific to the solid geometry and the viscoelastic model used. A third, recently proposed method also produces directly the time-dependent response but relies on the Laplace transforms of the fundamental solutions. Computer codes based on the different algorithms are developed and applied to benchmark problems in order to assess their relative accuracy and efficiency. Particular attention is given to the effectiveness of the methods to predict fracture parameters in cracked plate problems. The versatility, computational efficiency and accuracy of the different schemes are compared. In general, good agreement is achieved between various BEM predictions and other published numerical results. Schemes for possible extension of the method to account for more complex viscoelastic models are briefly discussed.

## 1 Introduction

The increasing demand of high quality materials in engineering design has led to an increasing use of polymers due to their high strength to weight ratio and to their corrosion resistance. Although polymers offer these advantages over traditional metallic materials, their characteristic time-dependent behaviour may lead to excessive creep and/or failure. Thus, the study of long-term polymer component behaviour under various loading conditions is becoming increasingly important.

Polymers are materials behaving according to a constitutive model known as viscoelasticity, which accounts for an interdependence of stress and strain with time. In order to study the response of viscoelastic solids to arbitrary, external, time-dependent loads, a numerical analysis is normally needed. Whereas the finite element method (FEM) remains the most popular numerical method today for solid material analysis, more recently, the boundary element method (BEM) has been developed as an effective alternative numerical technique. Although many studies on the application of BEM to static or dynamic viscoelastic problems can be found in the literature, a systematic assessment of the relative merits or limitations of the various approaches previously employed is apparently missing.

There are two main approaches to linear viscoelastic analysis by the BEM. The first method [1] uses the correspondence principle to generate an associated elastic problem, which is solved in the Laplace transformed domain and the result is inverted numerically so that the solution in the time domain is obtained. In this approach, numerical inversion is an additional task requiring attention in its implementation. The second, direct method [2] involves the formulation of a boundary integral equation in the time domain which is solved by a step-by-step time integration scheme. The need for the appropriate time-domain viscoelastic fundamental solution limits the power of this approach. A new method, recently proposed [3], seems to combine the advantages of the previous two, solving the problem in the time domain but relying on the fundamental solutions in the Laplace domain. This mixed method does not appear to be fully developed, neither its efficiency and accuracy have been thoroughly tested.

In this paper, quasi-static BEM analyses of polymers are briefly reviewed and developed computer codes based on different algorithms are applied to benchmark problems in order to assess their relative accuracy and efficiency. Particular attention is given to the analysis of cracked plates imposing additional computational requirements for the representation of stress singularities and the evaluation of stress intensity factor and the  $J$ -integral.

The Laplace transformed domain scheme has the advantage of relying on the fundamental solutions of the corresponding elasticity problems, it is therefore conceptually easy to extend its applicability to various types of solid analyses and a wide range of material models. It is shown that this, more versatile approach is computationally more demanding and its accuracy depends on the range and distribution of transform parameter values adopted.

The direct time domain formulation, using fundamental solutions specific to the solid geometry and the adopted viscoelastic model, requires the identification or determination of the appropriate fundamental solution but it proves computationally more efficient. Published time-dependent fundamental solutions for various cases are reviewed and the validity of some of them is theoretically and numerically confirmed. The potential of the mixed method to generate quasi-static solutions is explored with a preliminary investigation into the parameters controlling convergence. In general, good agreement is achieved between various BEM predictions and other published numerical results. Schemes for

possible extension of the methods to account for more complex viscoelastic models are briefly discussed.

## 2 Background theory

The linear viscoelastic model adopted in most BEM formulations is, in accordance with Boltzmann's principle, of hereditary integral type

$$\sigma_{ij} = G_{ijkl}(t)\varepsilon_{kl}(0) + \int_0^t G_{ijkl}(t-\tau) \frac{\partial \varepsilon_{kl}(\tau)}{\partial \tau} d\tau \quad (1)$$

where  $\sigma_{ij}$ ,  $\varepsilon_{ij}$  are the stress and small strain tensors, respectively, and  $G_{ijkl}(t)$  the relaxation moduli in the general case of an anisotropic medium. Adopting the notation for the Stieltjes convolution of two functions [4], eqn (1) can be more concisely written

$$\sigma_{ij} = G_{ijkl} * d\varepsilon_{kl} \quad (2)$$

In the case of an isotropic medium characterised by the moduli  $K(t)$  and  $\mu(t)$ , corresponding to the bulk and shear moduli in elasticity, the constitutive relations (2) can be transformed to

$$s_{ij} = 2\mu(t) * de_{ij}(t), \quad \sigma_{kk} = 3K(t) * d\varepsilon_{kk}(t) \quad (3)$$

where  $s_{ij}$  and  $e_{ij}$  are, respectively, the deviatoric stress and strain tensors. A commonly used rheological model is the generalised standard linear solid (SLS) [5]. It can be formed by connecting in series a Hookean spring and  $N$  Kelvin models, or by connecting in parallel a spring and  $N$  Maxwell models. The resulting viscoelastic equations are of differential operator type, the solution of which under relaxation or creep conditions leads to the determination of the time-dependent relaxation or creep moduli, respectively.

Introducing the small strain-displacement relations into the constitutive eqns (1) and substituting the latter into the stress equations of equilibrium yields a system of integro-differential equations

$$G_{ijkl}(t)u_{k,lj}(0) + \int_0^t G_{ijkl}(t-\tau) \frac{\partial u_{k,lj}(\tau)}{\partial \tau} d\tau + f_i = 0 \quad (4)$$

where  $f_i$  is the body force per unit volume. The problem is complemented by the boundary conditions

$$u_i(t) = \tilde{u}_i(t) \text{ on } \Gamma_1 \quad \sigma_{ij}(t)n_j = \tilde{p}_i(t) \text{ on } \Gamma_2 \quad (5)$$

where  $\mathbf{n}$  is the outward unit normal vector to the boundary  $\Gamma = \Gamma_1 + \Gamma_2$ .

Given two viscoelastic states  $(u_i, p_i, f_i)$  and  $(u_i^*, p_i^*, f_i^*)$ , satisfying the boundary value problem described above, the reciprocity relation [4]

$$\int_{\Gamma} p_i * du_i^* d\Gamma + \int_{\Omega} f_i * du_i^* d\Omega = \int_{\Gamma} u_i * dp_i^* d\Gamma + \int_{\Omega} u_i * df_i^* d\Omega \quad (6)$$

can be derived. The alternative form

$$\int_{\Gamma} p_i * u_i^* d\Gamma + \int_{\Omega} f_i * u_i^* d\Omega = \int_{\Gamma} u_i * p_i^* d\Gamma + \int_{\Omega} u_i * f_i^* d\Omega \quad (7)$$

involving Riemann convolutions can be shown to be also valid.

Taking the Laplace transform of both sides of constitutive eqns (1) gives

$$\bar{\sigma}_{ij} = s\bar{G}_{ijkl}\bar{\varepsilon}_{kl} = G_{ijkl}^L \bar{\varepsilon}_{kl} \quad (8)$$

By transforming also the equations of equilibrium (4), the strain-displacement relations, as well as the boundary conditions (5), a complete correspondence is established between the elastic and the linear viscoelastic problem. The latter can thus be solved in the transformed domain for any range of values of the transform variable  $s$  by the same methods as those applicable to the corresponding elasticity problem. In the end, it is, of course, necessary to obtain the solution in real time through inversion of the transform so obtained. This, so called, correspondence principle has been applied directly to generate BEM solutions of the transformed physical problem but also to obtain the fundamental solutions for particular viscoelastic models, which are then used in time domain BEM formulations.

### 3 BEM formulations

#### 3.1 Laplace transformed domain

If the correspondence principle is applied to the quasi-static problem, a BEM solution can be developed from the boundary integral equation in the Laplace transformed domain

$$\kappa_{ij}\bar{u}_i = \int_{\Gamma} [\bar{p}_i(s)u_{ij}^*(s) - \bar{u}_i(s)p_{ij}^*(s)]d\Gamma + \int_{\Omega} \bar{f}_i u_{ij}^* d\Omega \quad (9)$$

where  $\kappa_{ij} = 0.5\delta_{ij}$  in the case of a smooth boundary, and  $(u_{ij}^*, p_{ij}^*)$  is the elastic fundamental solution for displacements and tractions in which however the elastic constants have been replaced by the corresponding functions in the transformed space according to eqn (8). The calculated Laplace transforms of boundary or domain variables can be numerically inverted back into time-dependent functions using any of the available numerical inversion methods.

#### 3.2 Time domain

The boundary integral equation can be obtained directly from the reciprocal theorem of linear viscoelasticity (6). This is achieved by choosing the system  $(u_i^*, p_i^*, f_i^*)$  to coincide with the fundamental solution of the viscoelastic problem, that is, the displacements  $u_{ij}^*(\mathbf{x}-\xi, t)$  and tractions  $p_{ij}^*(\mathbf{x}-\xi, t)$  generated by unit body forces in each co-ordinate direction applied at  $\mathbf{x}=\xi$  and time  $t=0$ . These unit forces, represented by

$$f_{ij}^* = \delta_{ij}\delta(\mathbf{x}-\xi)H(t)$$

where  $\delta_{ij}$  is the Kronecker delta,  $\delta(\mathbf{x}-\xi)$  the delta function and  $H(t)$  the Heaviside step function, are substituted into eqn (6), which then provides, for a point  $\xi$  on the boundary of  $\Omega$ :

$$\kappa_{ij}u_i(t) = \int_{\Gamma} (p_i * du_{ij}^* - u_i * dp_{ij}^*) d\Gamma + \int_{\Omega} f_i * du_{ij}^* d\Omega \quad (10)$$

or, taking into account a property of the Stieltjes convolution [4],

$$\kappa_{ij}u_i(t) = \int_{\Gamma} (u_{ij}^* * dp_i - p_{ij}^* * du_i) d\Gamma + \int_{\Omega} f_i * du_{ij}^* d\Omega \quad (11)$$

The inverse Laplace transform of the elastic fundamental solution in the transformed space is required in the above time domain formulation. Such an operation has been carried out in several special cases. Carini and De Donato [5] obtained the fundamental solutions for a general Kelvin or Maxwell SLS model.

### 3.3 Mixed formulation

A particular mixed scheme [3] was based on the boundary integral equation

$$\kappa_{ij} * u_i(t) = \int_{\Gamma} (u_{ij}^* * p_i - p_{ij}^* * u_i) d\Gamma + \int_{\Omega} f_i * u_{ij}^* d\Omega \quad (12)$$

which can be obtained from the reciprocity relation (7) if the fundamental solution  $u_{ij}^*(\mathbf{x}-\xi, t)$ ,  $p_{ij}^*(\mathbf{x}-\xi, t)$ , due to the body force

$$f_i^* = \delta_{ij} \delta(\mathbf{x}-\xi) \delta(t) \quad (13)$$

is used as the second viscoelastic state. If time  $t$  is divided into  $N$  equal intervals  $\Delta t$  so that  $t = N\Delta t$ , the convolution integrations in eqn (12) may be performed by the convolution quadrature method proposed by Lubich [6, 7]. This quadrature formula uses integration weights depending only the Laplace transformed functions  $u_{ij}^*$  and  $p_{ij}^*$ . Thus a time stepping procedure can be formulated directly in the time domain, although only the Laplace transforms of the fundamental solutions are used, that is, a viscoelastic boundary element formulation in the time domain is achieved without requiring the knowledge of the time dependent fundamental solutions.

## 4 Boundary element modelling

Constant boundary elements were used in the present numerical implementations of BEM formulations in both the transformed and time domain. Time domain formulations based on integral equations (10), (11) or (12) require modelling also in the time dimension. If the boundary surface  $\Gamma$  is discretised in  $E$  elements  $\Gamma_e$ , the following representation can be adopted,

$$u_j(\mathbf{x}, t) = u_j^e(t), \quad p_j(\mathbf{x}, t) = p_j^e(t) \quad (14)$$

where  $u_j^e(t)$  and  $p_j^e(t)$  are the time dependent nodal values of displacement and traction, respectively.

Boundary integral equation (11) was discretised assuming that the boundary variables  $u_i(\mathbf{x}, t)$  and  $p_i(\mathbf{x}, t)$  are linear with respect to time  $t$  within a small time step  $\Delta t_\kappa = t_\kappa - t_{\kappa-1}$  and the viscoelastic fundamental solutions have the general form:

$$p_{ij}^* = a_{ij}^0(x, \xi) + \sum_{m=1}^M a_{ij}^m(x, \xi) e^{-\alpha_m t}, \quad u_{ij}^* = b_{ij}^0(x, \xi) + \sum_{n=1}^N b_{ij}^n(x, \xi) e^{-\beta_n t} \quad (15)$$

The discretised form of eqn (11) was obtained as

$$\begin{aligned} \kappa_{ij}(\xi) u_i^{(K)}(\xi) &= \sum_{n=0}^N B_j^{n(K)}(\xi) + \sum_{\kappa=1}^K \sum_{n=1}^N [B_j^{n(\kappa-1)}(\xi) e^{-\beta_n(t_\kappa - t_{\kappa-1})} (e^{-\beta_n \Delta t_\kappa} - 1)] \\ &\quad - \sum_{m=0}^M A_j^{m(K)}(\xi) - \sum_{\kappa=1}^K \sum_{m=1}^M [A_j^{m(\kappa-1)}(\xi) e^{-\alpha_m(t_\kappa - t_{\kappa-1})} (e^{-\alpha_m \Delta t_\kappa} - 1)] \end{aligned} \quad (16)$$

where, for simplicity, the body force is assumed to be zero and

$$\begin{aligned} A_j^{m(\kappa)}(\xi) &= \int_{\Gamma} a_{ij}^m(x, \xi) u_i^{(\kappa)}(x) d\Gamma, \quad B_j^{n(\kappa)}(\xi) = \int_{\Gamma} b_{ij}^n(x, \xi) p_i^{(\kappa)}(x) d\Gamma \\ u_i^{(\kappa)}(x) &= u_i(x, t_\kappa), \quad p_i^{(\kappa)}(x) = p_i(x, t_\kappa) \end{aligned}$$

It is evident from eqn (16) that the boundary displacements and tractions can be determined at any time  $t = t_\kappa$  if they are known at all previous times. At  $t = 0$  all unknown boundary values can be calculated when the boundary integral equation (10) governs only the initial elastic response due to any non-zero initial values of the boundary or loading conditions. At any following time  $t = t_\kappa$  the respective unknown boundary values can be obtained from eqn (16) with the current boundary conditions and the additional terms depending only on the solution at the previous steps. A step-wise procedure is thus established which advances the solution until the final time step is reached. After the unknown boundary values of the linear viscoelastic problem are determined, the displacements and stresses at internal points can be calculated using expressions obtained from eqn (10) with  $\kappa_{ij} = \delta_{ij}$ .

The numerical algorithm for the mixed method is obtained by inserting the boundary models (14) in eqn (12) with the body forces neglected. This gives

$$\kappa_{ij}^* u_i(t) = \sum_{e=1}^E \left\{ \int_{\Gamma_e} u_{ij}^*(x, \xi; t) * p_j^e(t) d\Gamma_e - \int_{\Gamma_e} p_{ij}^*(x, \xi; t) * u_j^e(t) d\Gamma_e \right\} \quad (17)$$

Applying the quadrature formula proposed by Lubich to the integral equation (17) results in the following boundary element time-stepping formulation for  $n = 0, 1, \dots, N$ ,

$$\sum_{k=0}^n \omega_{n-k}(\bar{\kappa}_{ij}^*) u_j(k\Delta t) = \sum_{e=1}^E \sum_{k=0}^n \left\{ \omega_{n-k}(\bar{u}_{ij}^*) p_j^e(k\Delta t) - \omega_{n-k}(\bar{p}_{ij}^*) u_j^e(k\Delta t) \right\} \quad (18)$$

with the spatial integration incorporated into the weights  $\omega_n$  which are approximately given by

$$\omega_n(\bar{g}_{ij}^*, \xi, \Delta t) = \frac{1}{L} \sum_{l=0}^{L-1} \left[ \int_{\Gamma_e} \bar{g}_{ij}^*(x, \xi, \frac{\gamma(z_l)}{\Delta t}) d\Gamma \right] z_l^{-n}$$

where function  $g$  represents  $u_{ij}^*(t)$  or  $p_{ij}^*(t)$ ,  $\gamma(z)$  is an analytic function, which should satisfy certain stability criteria as postulated by Lubich and  $z_l = \rho e^{i(2\pi l/L)}$ ,  $\rho$  being the radius of a circle within the domain of analyticity of  $u_{ij}^*$  and  $p_{ij}^*$ . Thus an algebraic system of equations for the discrete nodal values  $p_{ij}^*(k\Delta t)$  and  $u_{ij}^*(k\Delta t)$  is formed with coefficients depending on the Laplace transforms of the fundamental solutions  $u_{ij}^*(x, \xi, t)$  and  $p_{ij}^*(x, \xi, t)$ .

## 5 Numerical results

In order to test the reliability of the developed computer programs, several problems were solved, including an infinite plane with a circular hole, as well as a thick walled cylinder with and without an outside elastic ring. The applied load was constant internal pressure in all cases. All these analyses gave numerical results in very good agreement with the corresponding exact solutions.

Numerical results from the methods described in the previous sections are presented for the problem of the thick wall cylinder reinforced by an elastic ring as shown in Fig. 1. Initially there is no traction or gap between the cylinder and the ring; then the inner boundary  $L_1$  of the cylinder is subject to a uniform pressure  $p = 100$  MPa applied as a step load at time  $t = 0$ . The numerical values used are  $a = 6$  mm,  $b = 20$  mm and  $h = 1$  mm. The adopted viscoelastic material model is that assumed by previous investigators for the same problem [1, 8], namely, elastic behaviour in bulk deformation with  $K = 128$  GPa and standard linear solid in shear according to

$$\mu(t) = 12 + 36e^{-0.4t} \text{ (GPa)} \quad (19)$$

where the constants can be easily related to the properties of either a Kelvin or a Maxwell model. The material values chosen are those used by Sim and Kwak [8]. The Young's modulus of the elastic ring is 207 GPa, and the Poisson's ratio is 0.25.

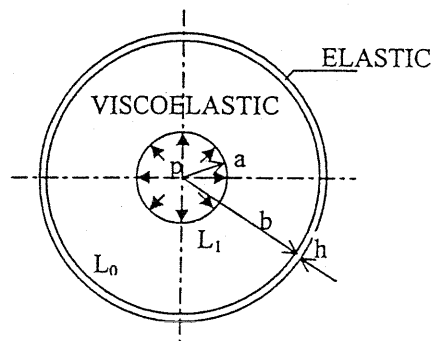


Figure 1: Thick wall cylinder reinforced by an elastic ring.

Taking advantage of symmetry, only one quarter of the cylinder was analysed. The boundary meshes for both methods were the same consisting of boundary elements of more or less uniform length. BEM analyses were

performed under both plane strain and plane stress conditions. In the transform method, Schapery's inversion method [1] was used with 30 discrete values for the transform parameter  $s$ , satisfying  $s_{r+1} = 2s_r$ ,  $r = 1, 2, \dots, 29$  with  $s_1 = 0.001$ . In the direct method, the time step was kept constant at  $\Delta t_x = 0.5$  s.

Numerical time histories of the circumferential stress at various radial locations were found in excellent agreement with the exact solution predictions. Table 1 shows the average error for two boundary element meshes, where  $N_{BE}$  is the number of BEs. It can be seen that, for the chosen modelling parameters, the direct method is generally more accurate than the transform method. It is worth noting that refining the mesh around corners contributed significantly to the improvement of the accuracy of the results achieved by increasing the number of boundary elements. Table 1 is based on results obtained under plane strain conditions but very similar trends were observed in the results from the plane stress case.

Table 1: Numerical error in circumferential stress calculations

Radial co-ordinate $r$ (mm)	$N_{BE} = 88$		$N_{BE} = 275$	
	Transformed domain	Time domain	Transformed domain	Time domain
6.5	2.46 %	3.05 %	0.26 %	0.16 %
13.5	0.11 %	-0.06 %	0.06 %	0.01 %
19.5	0.94 %	0.58 %	-0.24 %	-0.23 %

New BEM results were obtained in the case of a long strip with a central crack under uniform lateral extension. Accounting for symmetry with respect to both  $x$  and  $y$  axes, only one quarter of the plate was analysed as shown in Fig. 2. This was a model of a specimen used for studying crack propagation in a viscoelastic solid [9]. The material was assumed to have a constant Poisson's ratio  $\nu = 0.4$  and a standard linear solid behaviour in shear

$$\mu(t) = 1.057 + 154.3e^{-5t} \text{ (MPa)} \quad (20)$$

This material model does not represent accurately the time dependence of the material tested Mueller and Knauss [9] but does give the quoted extreme values of relaxation modulus at  $t = 0$  and  $t = \infty$ . A lateral extension  $u_y = 0.2$  mm was uniformly applied along the edge  $y = 17.46$  mm. The BEM model consisted of 534 BEs the majority of which were located in the neighbourhood of the crack tip.

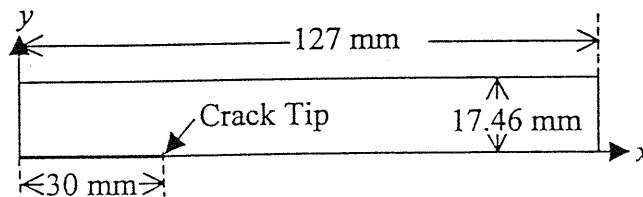


Figure 2: Centrally cracked long strip



Both time and transformed domain results for the time-dependent stress concentration factor  $K_I(t)$  are plotted in Fig. 3. These were obtained using

$$K_I(t) = \lim_{r \rightarrow 0} \sigma_{yy}(r, t) \sqrt{2\pi r} \quad (21)$$

where  $r = x - 30$  (mm) is the distance from the crack tip. The limit on the right hand side of eqn (21) was identified by linear regression since, theoretically, the corresponding expression is represented by a straight line. Although the agreement between the two BEM solutions at  $t = 0$  is very good, considerable deviation is observed at later times. This can be attributed to the insufficient number of Laplace transform solutions. The extreme BEM time domain results  $K_I(0) = 20.89 \text{ Nmm}^{-3/2}$  and  $K_I(\infty) = 0.1420 \text{ Nmm}^{-3/2}$  can be compared with the theoretical predictions for an infinite strip which are 22.72 and 0.1545, respectively [9]. The error of about 8% could be partly numerical but mainly due to the difference between infinite and finite dimensions.

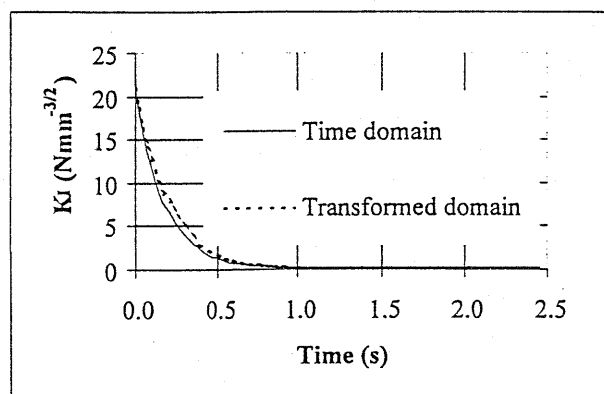


Figure 3: Stress intensity factor for the strip problem.

## 6 Discussion and conclusions

The transformed domain method is certainly more versatile since it can be adapted to any type of viscoelastic model but requires the transform inversion and the associated choice of range and distribution of the transform parameter, both having a strong influence on the accuracy of the final results. Increasing the number of Laplace transformed solutions imposes a heavy computational penalty on the final output. With regard to viscoelastic fracture mechanics problems, this method allows the determination of the stress intensity factor through a path-independent integral in the transformed domain [10], similar to that defined in linear elastic fracture mechanics.

The time domain method yields directly time histories of results, it has therefore proved to be more efficient than the transformed domain method. Another advantage of the time domain method is that it can handle more easily

inputs of complex time histories of loading conditions. However, the time-dependent fundamental solution for the adopted viscoelastic model must be available. Although such solutions exist for a wide range of cases [5], their numerical implementation remains a challenge due to the complexity of their general form. This disadvantage may be overcome by exploring further the mixed method proposed by Schanz [3]. Before extending its application to quasi-static problems, ranges of parameters guaranteeing convergence should be firmly established. Preliminary assessments of its potential have shown that its accuracy and stability depend on an appropriate choice of the approximation parameters  $\Delta t$ ,  $\rho$  and  $L$ , as described in Section 4. Numerical results will hopefully show that this method can be accepted as a versatile alternative to the other two in most cases.

There is considerable scope for increasing the potential of the method to solve complex viscoelastic problems. This can be achieved by enhancing its range of material modelling and extending its applicability to complex, industry-oriented problems. One such objective is the analysis of non-linear viscoelastic behaviour, which can be more important especially for long-term, high stress concentration situations. This can be achieved through an extension of the time domain approach, which however needs to become more versatile by incorporating the widest range possible of available time-dependent fundamental solutions.

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