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EFFICIENT BOUNDARY ELEMENT FORMULATION OF THERMOELASTICITY

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Abstract. *The problem of thermoelasticity is present in many different areas of solid mechanics. It describes the effects of thermal as well as mechanical loads on an elastic structure. We use the uncoupled quasistatic formulation of thermoelasticity (UQT), in a linear model and apply the Boundary Element Method. The UQT formulation is applicable in most cases, where the mechanical load is constant or slowly varying in time. Here, the influence of the elastic deformations on the heat distribution is neglected. This leaves us with a decoupled system of differential equations, consisting of the heat equation and an elastic equation, which accounts for thermal and mechanical loads. In the elastic equation the thermal field variables are introduced via convolutions. We apply three different methods for the calculation of these convolutions to find the elastic field variables and compare their computation times.*

1 INTRODUCTION

For a large class of problems in solid mechanics not only mechanical loads but also thermal influences have to be considered to describe the behavior of a structure correctly. For an elastic deformation under the influence of heat, the theory of thermoelasticiy is well known for over 5 decades (see for example [1–3]). Today we can apply the theory in many different fields, for example in structural engineering or in the description of a hot forming tool. This tool is used in the production of vehicle parts. The process of hot forming makes use of the thermomechanical properties of the material. In the process, the tool is directly heated and cooled down thereafter. For this industrial application the thermal problem has been simulated and a fast method was developed in a previous work by Messner and Schanz [4]. It is work in progress to extend this thermal problem to the elastic deformations, caused by the temperature change.

Therefore, in our studies we aim to develop a fast numerical method to calculate the effect of such thermomechanical loads and to simulate the elastic deformations. The model we use is linear in its geometry, as well as in its elastic and thermal behavior and thus applicable only to small deformations. For this purpose the Boundary Element Method (BEM) is a good framework for our numerical model. In the BEM the discretization of the body is reduced to a discretization of the body's surface. Results at an arbitrary point of the volume can be calculated in a subsequent step. In particular, we use the theory of Uncoupled Quasistatic Thermoelasticity (UQT), which is a special case of thermoelasticity that meets the requirements of our applications. The UQT has been studied [3, 5, 6] and applied by different authors (see [7, 8]).

In the following, we will describe the theoretical approach we use and the different methods to solve the equations. We show numerical results and compare them to a known analytic solution. Additionally, we present a comparison of computation times for these results.

2 BASIC EQUATIONS

The general case of coupled thermoelasticity can be described by the following set of coupled differential equations [6]

$$\kappa\,\theta_{,jj} - \dot{\theta} - \kappa\,\alpha\,\dot{u}_{j,j} + \psi = 0 \tag{1}$$
$$\mu\,u_{i,jj} + (\lambda+\mu)\,u_{j,ij} - (3\lambda+2\mu)\,\alpha\,\theta_{,i} + f_i = \rho\,\ddot{u}_i \quad , \tag{2}$$

with

u_i	displacement	λ, μ	Lamé isothermal elastic constants
θ	temperature	α	thermal expansion coefficient
f_i	body forces	κ	thermal diffusivity
ψ	body heat sources	ρ	mass density.

For this set of coupled differential equations, a simplification can be justified, which applies to many technical applications. In a process of slowly varying mechanical load, the heat production or consumption due to mechanical stress can be neglected. For such a slow or quasistatic process the elastic inertia terms can be neglected as well. With these assumptions we end up with the set of uncoupled quasistatic differential equations of thermoelasticity (in the following denoted by UQT) [5], where the term describing the influence from mechanical stress on the heat evolution vanishes. Additionally, we do not consider body forces or inner heat sources in this model

$$\kappa\,\theta_{,jj} - \dot{\theta} \;=\; 0 \tag{3}$$
$$\mu\,u_{i,jj} + (\lambda+\mu)\,u_{j,ij} - (3\lambda+2\mu)\,\alpha\,\theta_{,i} \;=\; 0 \quad . \tag{4}$$

With this set of equations, the thermal evolution in equation (3) is completely independent, or uncoupled, from the mechanical variables. This provides us with the possibility to solve this differential equation independently. As a result, the thermal quantities are determined and are known in advance for the solution of the elastic differential equation (4), where they can be considered as a thermal load.

To apply the Boundary Element Method we need to formulate boundary integral equations for this set of differential equations, which are [7]

$$c_{\theta\theta}(\xi)\,\theta(\xi,t) \;=\; \int_\Gamma \{\,[g_{\theta\theta} * q](x,t) - \,[f_{\theta\theta} * \theta](x,t)\}\;d\Gamma \tag{5}$$
$$c_{ij}(\xi)\,u_j(\xi,t) \;=\; \int_\Gamma \{\,g_{ij}t_j(x,t) - f_{ij}u_j(x,t) + \,[g_{i\theta} * q](x,t) - \,[f_{i\theta} * \theta](x,t)\}\;d\Gamma \;, \tag{6}$$

where $i, j = 1, 2, 3$. The functions g and f are the fundamental solutions, which can be found in [1, 3, 6]. While the purely thermal equation (5) is scalar, the elastic equation (6) is vectorial. The jump terms $c_{\theta\theta}$ and c_{ij} follow from shifting the field point ξ from the domain Ω to the boundary Γ.

In our studies, we will focus on the numerical solution of the elastic equation (6), since a fast method for the thermal equation (5) already exists [4].

Spatial Discretization

For a numerical description of our problem we need discretizations of both, space and time. The geometry description is based on an element formulation, establishing the Boundary Element Method. This method uses the triangulation of the geometry, yielding disjoint, adjacent, finite elements τ_l on the boundary Γ

$$\Gamma \approx \Gamma_L = \sum_{l=0}^{L} \tau_l \quad . \tag{7}$$

In contrast to other element methods, for the BEM the discretization of the surface Γ is sufficient, due to the boundary integral equations used. As a consequence, the volume description only depends on the quality of the surface description. The field $y(x,t)$ to be investigated is formed by a linear combination of shape functions $\phi(x)$. Depending on the choice of the shape functions, the physical quantity is determined by a sum over element functions ϕ_n and nodal values y_n,

$$y(x,t) = \sum_{n=0}^{N} \phi_n(x)\;y_n(t) \quad , \tag{8}$$

where N is the number of shape functions. The field variable y represents all four fields of interest, the displacement u_i, the temperature θ, the tractions t_i and the heat flux q.

3 TREATMENT OF THERMAL QUANTITIES

In the elastic equation, the thermal variables are introduced via convolutions over time. The boundary integral equation (6) convolves known boundary values with the fundamental solutions of the coupling terms as a right hand side. The treatment of these convolutions can be of different kind.

3.1 Analytic integration in time

We introduce discrete time steps

$$t_m = m\Delta t \qquad m = 0, 1, ..M \tag{9}$$

and shape functions $\psi_m(t)$ in time. The field is consequently a linear combination of these time shape functions

$$y_n(t) = \sum_{m=0}^{M} \psi^m(t)\, y^m \quad , \tag{10}$$

where M denotes the number of contributing time shape functions. Inserting these shape functions in the first convolution integral in 6, yields

$$\int_0^t g_{i\theta}(x, t-\tau) q(x,\tau)\, d\tau = \sum_{m=1}^{M} \int_{(m-1)\Delta t}^{m\Delta t} g_{i\theta}(x, M\Delta t - \tau)\, q^m(x) \psi^m(t)\, d\tau \,. \tag{11}$$

Choosing constant discontinuous shape functions in time results in variables, which are only dependent on the present interval. As a consequence, it becomes possible to pull out the field quantity from the time integral [7]. An analytic integration of the fundamental solutions is favorable. It exists for the heat-coupling fundamental solution and was developed by Dargush [7]. With these assumptions the convolution involves only the multiplication of matrices and boundary value vectors

$$\begin{aligned} \int_0^t g_{i\theta}(x, t-\tau) q(x,\tau)\, d\tau &= \sum_{m=1}^{M} q^m(x) \int_{(m-1)\Delta t}^{m\Delta t} g_{i\theta}(x, M\Delta t - \tau)\, d\tau \\ &= \sum_{m=1}^{M} q^m(x)\, G_{i\theta}^{M+1-m}(x) \,, \end{aligned} \tag{12}$$

where $G_{i\theta}$ is the time integrated fundamental solution. A triangular block Toeplitz structure is formed. This is a convenient method involving nothing but variables in the time domain.

3.2 The Convolution Quadrature Method (CQM)

The Convolution Quadrature Method was developed by Lubich [9, 10], to numerically evaluate a convolution, making use of one of the functions in the Laplace domain. The basic idea of the CQM is to express the convolution as a quadrature formula. The weights are derived from one of the function's Laplace transform

$$\mathcal{L}\{g\}(s) = G(s) = \int_0^\infty g(t)\, \mathrm{e}^{-st}\, dt \quad . \tag{13}$$

The entire derivation of the CQM is shown in the Appendix. The strategy leads to the following formulation. First, we discretize in time

$$t_n = n\Delta t \quad , \tag{14}$$

with $n = 0, 1, ..., N$, for the discrete convolution of $N + 1$ time intervals of equal size. Hence, it is

$$\int_0^t g_{i\theta}(x, t-\tau) q(x,\tau)\, d\tau \approx \sum_{k=0}^{n} \omega_{n-k}(\Delta t) q(k\Delta t) \quad . \tag{15}$$

$\omega_n(\Delta t)$ depends on the Laplace transform of the function, $G_{i\theta}(\frac{\gamma(z)}{\Delta t})$, where $\gamma(z)$ is the characteristic function of the underlying multistep method.

3.3 Fast Fourier Transformation (FFT)

The Fourier transform is another method which shifts the problem to the frequency domain, where the convolution becomes simply a multiplication

$$\mathcal{F}\{g * q\}(\omega) = \mathcal{F}\{g\}(\omega)\, \mathcal{F}\{q\}(\omega) = Y(\omega) \quad . \tag{16}$$

Here $\mathcal{F}$ denotes the Fourier transformation of the form

$$\mathcal{F}\{g\}(\omega) = G(\omega) = \frac{1}{\sqrt{2\pi i}} \int_{-\infty}^{\infty} g(t)\, \mathrm{e}^{-i\omega t}\, dt \quad . \tag{17}$$

As the thermoelastic problem is causal, there is no solution at negative times, and the Fourier transformation becomes almost equivalent to the Laplace transform for setting the parameter $s = i\omega$.

Therefore, it is possible to make use of the fundamental solution, which exists for the Laplace domain in an analytic form, and use it for the transformation into Fourier space as well. Finally, an inverse Fourier transformation has to be applied to the product $Y(\omega)$, which yields the result $y(t)$ in time domain

$$\mathcal{F}^{-1}\{Y\}(\omega) = y(t) \quad . \tag{18}$$

For a numerical algorithm of the discrete Fourier transformation there exists the very efficient Fast Fourier Transform algorithm (FFT). It operates at an effort of order $O(N log N)$.

Even though all methods are given for one of the convolution integrals exemplary here, both convolution integrals in the elastic equation (6) are treated in the same way.

4 RESULTS

4.1 Problem Validation

To validate the results of the uncoupled quasistatic thermoelastic problem, we want to consider a test problem for which an analytic solution exists. In literature there exist several simple and well known problems for the solution of the heat equation alone but not so many with a simple thermoelastic solution as well. There is one popular test case which goes back to Timoschenko and Goodier [11] and was also used by Dargush [7] and Chatterjee [8] for validation.

The problem setting is the following. A cubic body of homogeneous, isotropic material properties is fixed by roller bearings on 5 of its faces. At these faces the heat flux is zero, thus the system is thermally insulated there. The remaining 6th face of the cube is mechanically unconstrained (figure 1). Initially, the cube is in an equilibrium state at zero degrees. At time

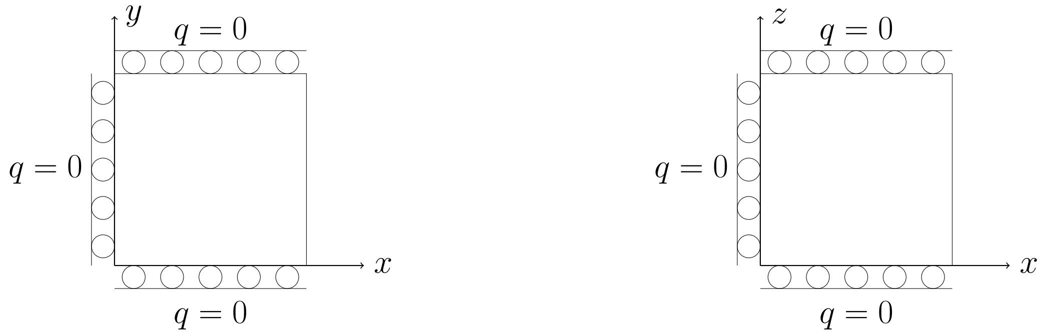

Figure 1: Mechanical and thermal constraints of the unit test cube, in top view and front view.

zero the temperature at the mechanically unconstrained face 6 is raised by 1 degree. As a result, the body expands elastically, as the temperature increases. After a certain time a stationary state is reached. Due to the mechanical boundary conditions the elastic expansion of the cube is only possible in x-direction. The three-dimensional model shows, therefore, a one dimensional behavior, for which solutions are known. The behavior is reduced to a one dimensional problem of the coordinate x with the following analytic solutions for the temperature θ and the displacement u

$$\theta(x,t) = 1 - \frac{4}{\pi} \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)} \quad \exp\left(- \frac{(2n+1)^2 \pi^2 \kappa\, t}{4L^2} \right) \quad \cos\left(\frac{(2n+1)\pi\, x}{2L} \right) , \tag{19}$$

$$\begin{aligned} u(x,t) &= \frac{(3\lambda + 2\mu)\alpha}{\lambda + 2\mu} \int_0^x \theta(x,t)\, \mathrm{d}y \\ &= \frac{(1+\nu)\alpha}{(1-\nu)} \left(x - \frac{8L}{\pi^2} \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)} \exp\left(- \frac{(2n+1)^2 \pi^2 \kappa\, t}{4L^2} \right) \sin\left(\frac{(2n+1)\pi\, x}{2L} \right) \right) , \end{aligned} \tag{20}$$

where L is the length of the cube in x-direction. With the relations of the Lamé coefficients of an isotropic material, the prefactor depends only on Poisson's ratio ν and the thermal expansion coefficient α.

For the following calculations the heat equation was solved in a first step, using the CQM. Since a fast method for the thermal problem exists, we want to focus on the deformations only. The elastic part was solved in a second step using the three different methods presented before for the convolution terms. Each method is going to be compared to the analytic solution of our test problem. As our test body, we choose the unit cube (figure 1), with its mechanically unconstrained face at $x = 1$. We show the elastic displacement over time for a point on this surface and denote the surface by $x = 1$.

Discretization The Boundary element mesh chosen for our surface approximation consists of triangular elements. The basic mesh has 24 elements, 4 triangles on each cube face. From this basic mesh 2 refinement levels are created, each splitting a previous element into 4 smaller triangles. In this manner, we receive refinement 1 with 96 boundary elements and refinement 2 of 384 elements. The meshes are shown in figure 2.

Time stepping For choosing an appropriate time step it is necessary to resolve the time dependence sufficiently. Therefore, the time step size highly depends on the material parameters,

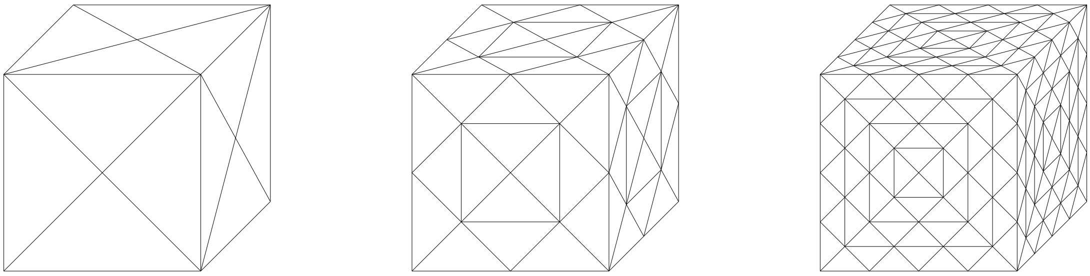

Figure 2: Basic mesh, refinement 1 and refinement 2.

especially on the thermal diffusivity κ and the heat expansion coefficient α. For the test case we choose the material parameters α and κ to be 1 and the Poisson's ratio ν to be zero. With these parameters a time step size of 0.01s is adequate.

Analytic integration in time (AIt)

As described in section 3.1, the fundamental solutions were analytically integrated for the elastic convolutions, which couple the heat quantities to the elastic deformations. The displacement u_x is shown for the basic mesh (24 elements), refinement 1 (96 elements) and refinement 2 (384 elements) and compared to the analytic solution, at a point on the free surface $x = 1$. In figure 3 a good agreement with the analytic solution is shown and in figure 4 convergence is observable.

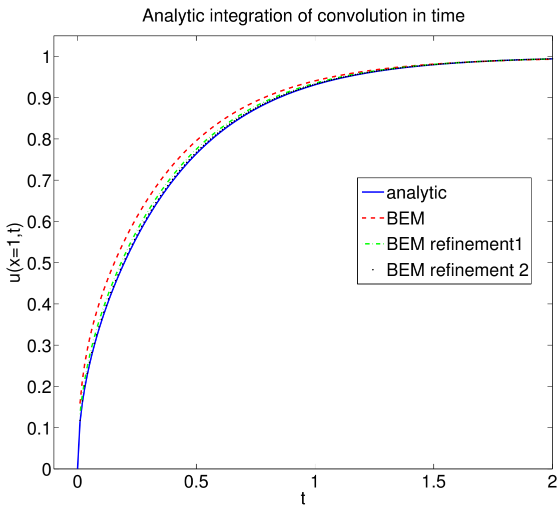

Figure 3: Convolution calculated by analytic integration with a time step size of Δt=0.01 seconds.

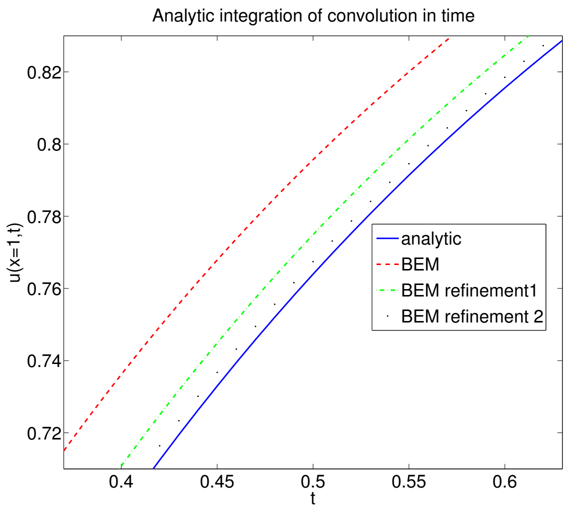

Figure 4: The zoom into the curve of figure 3 shows the convergence with the refinement.

Convolution Quadrature Method

The CQM yields high precision and convergence to the analytic solution as well. The quality is of the same order as for the analytic integration, for each mesh refinement, as shown in figures 5 and 6.

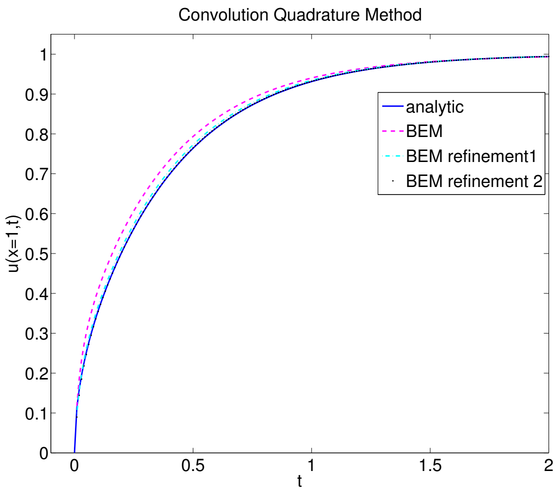

Figure 5: Displacement $u_x(x = 1)$, calculated using the CQM with Δt =0.01s.

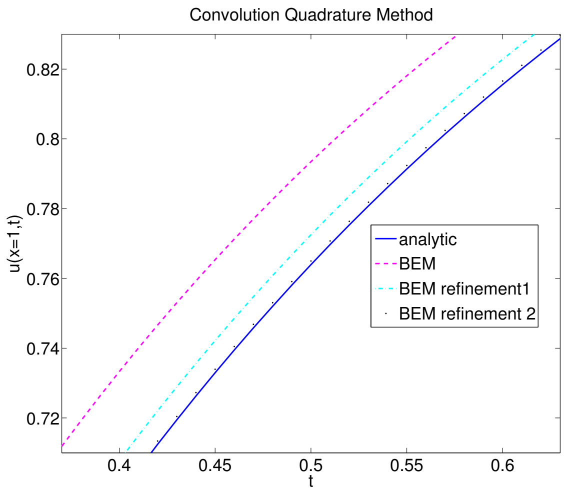

Figure 6: Zoom into figure 5 at around 0.5 seconds.

Fast Fourier Transformation

Calculating the elastic convolutions with the FFT, we once more receive results of comparable quality. The results for the test case are shown in figures 7 and 8.

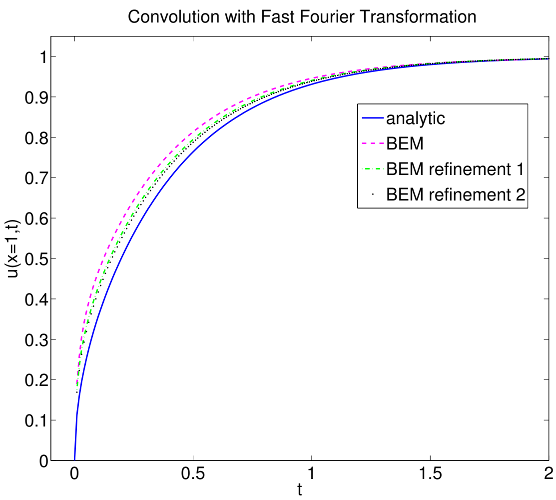

Figure 7: Displacement $u_x(x = 1)$, for the FFT convolution Δt =0.01s.

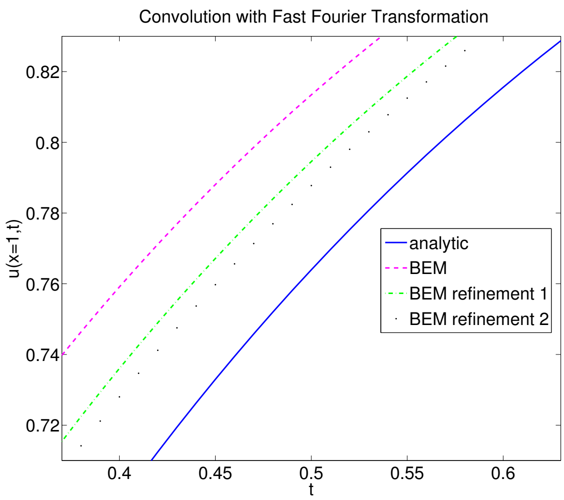

Figure 8: Zoom into figure 7 shows the convergence with the mesh refinement.

The result of refinement 2 is not as good as with CQM or the analytic integration method. This can be improved by choosing the parameters for the FFT differently.

Timings

Finally, we compare the computation time of the elastic equation for the three different methods of the convolution calculation. For each mesh refinement level the timings are shown, where AIt is our first method, which integrates the fundamental solutions analytically in time. The timings were taken on a standard PC using 6 cores. We use the parameters $\Delta t = 0.01$ seconds for the time step, for a total duration of 5 seconds.

	AIt	CQM	FFT
basic mesh	38	35	35
refinement 1	495	457	457
refinement 2	5921	5450	5250

Table 1: Comparison of computation times in seconds for the three convolution methods.

All three methods have similar computation times. The FFT is the fastest, followed by CQM and the analytic integration in time AIt, which is still fast.

5 CONCLUSIONS AND OUTLOOK

We showed the convergence of the displacement results to an analytic solution for the elastic equation of UQT, using three different methods for the convolution, an analytic integration, the CQM and the FFT. The results show a good agreement with the analytic solution, especially for high spatial discretization but already for quite coarse meshes as well. The time steps need to be chosen accordingly, depending on the thermal diffusivity and the heat expansion coefficient. Setting the material parameters to 1, we get a good resolution with Δt =0.01s. The computation time for the elastic equation is of the same order for all three methods. Still an even more efficient method is desirable, which accounts for the decrease of the rate of change of the field variables over time.

For time steps of variable sizes there exists the Generalized Convolution Quadrature Method (GCQM) introduced by Fernandez and Sauter [12]. We plan to apply this method to our problem. For the matrix assembling there are various fast methods available in the literature. It is work in progress to implement further methods for efficiency improvements.

A Appendix: CQM

The Convolution Quadrature Method was introduced by Lubich [9], in 1988 and has since been adapted by other authors such as Banjai and Sauter [13]. The following derivation of the CQM is taken from [14], where further details can be found.

We want to determine the convolution of two functions f and g

$$[f * g](t) = \int_0^t f(t-\tau)\, g(\tau)\, d\tau \quad . \tag{21}$$

The first step is to replace the function f by its inverse Laplace transformation $\hat{f}(s)$ like

$$\int_0^t f(t-\tau)\, g(\tau)\, d\tau = \frac{1}{2\pi i} \lim_{R\to\infty} \int_{c-iR}^{c+iR} \hat{f}(s) \underbrace{\int_0^t \mathrm{e}^s(t-\tau) g(\tau) d\tau}_{x(s,t)}\, ds \tag{22}$$

The term $x(s,t)$ can be interpreted as the solution of a differential equation of first order with zero initial condition

$$\frac{dx(s,t)}{dt} = sx(s,t) + g(t) \quad . \tag{23}$$

This differential equation can be solved by a linear multistep method in a discrete formulation. The introduction of $N+1$ discrete time steps of length Δt leads to a discrete formulation of our convolution

$$y(t_n) = \frac{1}{2\pi i} \lim_{R\to\infty} \int_{c-iR}^{c+iR} \hat{f}(s) x(s,t_n)\, ds \quad . \tag{24}$$

The solution of $x(s,t_n)$ by a linear multistep method, such as the Backward Differential Formula of order 1 or 2 (BDF1, BDF2), together with some reformulations, which can be found in [14], leads us to the following representation of $x(s,t_n) = x_n$ as a power series

$$\sum_{n=0}^{\infty} x_n z^n = \frac{1}{\frac{\gamma(z)}{\Delta t} - s} \sum_{n=0}^{\infty} g(t_n) z^n \quad , \tag{25}$$

where $\gamma(z)$ is the characteristic function of the chosen multistep method. Plugging x_n into the discrete convolution in equation (24)

$$\sum_{n=0}^{\infty} y_n z^n = \frac{1}{2\pi i} \lim_{R\to\infty} \int_{c-iR}^{c+iR} \hat{f}(s) \frac{1}{\frac{\gamma(z)}{\Delta t} - s} ds \sum_{n=0}^{\infty} g(t_n) z^n \ , \tag{26}$$

with $y(t_n) = y_n$, and applying the residue theorem gives

$$\sum_{n=0}^{\infty} y_n z^n = \hat{f}\left(\frac{\gamma(z)}{\Delta t}\right) \sum_{n=0}^{\infty} g(t_n) z^n \quad . \tag{27}$$

Since we are interested in the solution y_n of the convolution for every time step, we use Cauchy's integral formula for the coefficients of the power series

$$\omega_n(\Delta t) = \frac{1}{2\pi i} \int_{|z|=\rho} \hat{f}\left(\frac{\gamma(z)}{\Delta t}\right) z^{-n-1} dz \quad , \tag{28}$$

where ρ is the radius of analyticity of $\hat{f}\left(\frac{\gamma(z)}{\Delta t}\right)$. Each of the discrete solutions y_n can then be determined by a comparison of coefficients

$$\sum_{n=0}^{\infty} y_n z^n = \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} \omega_{n-k}(\Delta t) g(k\Delta t) z^n \quad , \tag{29}$$

resulting in

$$y_n = \sum_{k=0}^{n} \omega_{n-k}(\Delta t) g(k\Delta t) \tag{30}$$

for all discrete times $n = 0, 1, ..., N$. With this reformulation we gained a simple multiplication of the function g in time domain by weights, depending on the Laplace transform of the function f and the chosen linear multi-step method for the term $x(s,t_n)$.

A further reformulation has been introduced by Banjai and Sauter [13], which leads to a system of decoupled linear equations in the Laplace domain. By inserting the weights ω_n into equation (30) a representation as an inverse transformation of the CQM can be found. An engineering application of this can be found in [15].

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