Galerkin-based discretisation of infinite-dimensional dissipative dynamical systems

Michael Groß and Peter Betsch¹

Summary

In this paper, we will present a numerical comparison of three kinds of time discretisations for semi-discrete viscoelastodynamics. In the introduction, we explain our main goals and our present ingredients. Then, we explain the used formulation of dissipative dynamics. The next step is a finite element discretisation in space and time. And finally, we show the numerical example.

Introduction

Treading boundary-initial value problems as moving solid bodies numerically, a spatial discretisation using the finite element method is a standard procedure in mechanical engineering. The time discretisation, however, has been still often carried out by finite differences, although a finite element approximation of the time dimension is well-known since many years [1] and self-evident after using spatial finite elements. For example, one advantage of finite elements in time is that one obtains a higher order accurate time approximation in a natural way. Since the last decade, finite elements in time are again in the researchers' interest, because a further advantage is that continuous temporal finite element methods inherit conservation laws of dynamical systems [2]. These methods are therefore a natural starting point to construct higher order energy-momentum conserving time integrators which turned out to be well suited for computing long time runs in nonlinear elastodynamics [3]. Second order conserving integrators are well-known to exhibit superior stability properties which are of utmost importance in a nonlinear finite element framework.

On the theoretical side, our goal is a unified description of dissipative dynamical systems. Important examples are viscoelasticity with dissipation of memory type, which we consider in this paper, viscoelasticity with dissipation of rate type and thermal dissipation. On the numerical side, we aim at a physically consistent discretisation to obtain more stable numerical schemes. Considering finite motions of a solid body consisting of viscoelastic material, we show that an energy consistent time integration is also of great advantage for dissipative dynamical systems. In contrast to the application of standard time integrators, the dissipation is guaranteed independent of the material parameters and not dependent on the time step

¹Chair of Computational Mechanics, Department of Mechanical Engineering, University of Siegen, Germany.

size. Our present ingredients are a Hamiltonian formulation of dissipative dynamics, which leads to weak evolution equations for all state variables. These equations are then discretised by standard finite elements in space and by standard, respectively, energy-momentum consistent finite elements in time.

Constitutive formulation

For viscoelasticity of memory type, we use an internal variable formulation. The starting point is a free energy $\Psi = \Psi(C_t, \Gamma_t)$ depending on the right Cauchy-Green tensor $C_t = F_t^T F_t$ and a tensor-valued internal variable Γ_t . Both the deformation mapping $\varphi_t \in L^2(B_0, \mathbb{R}^{n_{\text{dim}}})$ and the internal variable $\Gamma_t \in L^2(B_0, \mathbb{R}^{n_{\text{dim}} \times n_{\text{dim}}})$ are mappings from the reference configuration into Euclidean spaces. The deformation gradient is given by $F_t = \nabla \varphi_t$. The evolution equation of the fading memory $\dot{\Gamma}_t = f^{\text{mem}}(C_t, \Gamma_t)$ is chosen such that the second law of thermodynamics is fulfilled:

$$-\frac{\partial\Psi}{\partial\Gamma_t}:\dot{\Gamma}_t \ge 0 \tag{1}$$

We restrict us to isotropic finite viscoelasticity according to [4]. In this formulation, the free energy is divided into an equilibrium part and a non-equilibrium part: $\Psi = \Psi^{eq}(I_{C_t}, II_{C_t}, III_{C_t}) + \Psi^{neq}(I_{C_t^e}, III_{C_t^e})$. The equilibrium part of the free energy then depends on the invariants of the right Cauchy-Green tensor and the nonequilibrium part depends on the invariants of the so-called elastic right Cauchy-Green tensor defined by $C_t^e = C_t \Gamma_t^{-1}$. The evolution equation of the fading memory $\dot{\Gamma}_t \Gamma_t^{-1} = 2 \left[\mathcal{V}^{-1} : M_t^e \right]$ is chosen such that the Clausius-Duhem Inequality is given by a positive definite quadratic form with respect to the elastic Mandel stress tensor $M_t^e = [C_t^e]^T S_t^e$, where

$$S_t^e = 2 \frac{\partial \Psi^{\text{neq}}}{\partial C_t^e}$$
 and $\mathcal{V}^{-1} := \frac{1}{2\eta_{\text{dev}}} I^{\text{dev}} + \frac{1}{3\eta_{\text{vol}}} I^{\text{vol}}$ (2)

denotes the elastic stress tensor and the inverse viscosity tensor, respectively.

Dynamical Formulation

We use a Hamiltonian formulation in which the internal variable Γ_t is incorporated in the dynamics as a further state variable by defining the extended state manifold $X = Q \times V_Q \times S$ with the state variables $\varphi_t \in Q$, $\pi_t = \rho_0 V_t \in V_Q$ and $\Gamma_t \in S$. For functionals $\mathcal{F}, \mathcal{G} : X \to \mathbb{R}$ on X, there exists a bracket structure $\{\{\bullet, \bullet\}\}$ which is divided into two parts as follows: $\{\{\mathcal{F}, \mathcal{G}\}\} = \{\mathcal{F}, \mathcal{G}\} - \prec \mathcal{F}, \mathcal{G} \succ$, for all $\mathcal{F}, \mathcal{G} : X \to \mathbb{R}$. The first part is a Poissonian (skew-symmetric) bracket representing the conservative structure given by

$$\{\mathcal{F},\mathcal{G}\}(\varphi_t,\pi_t,\Gamma_t) = \int_{B_0} \frac{\delta\mathcal{F}}{\delta\varphi_t} \cdot \frac{\delta\mathcal{G}}{\delta\pi_t} - \frac{\delta\mathcal{F}}{\delta\pi_t} \cdot \frac{\delta\mathcal{G}}{\delta\varphi_t}$$
(3)

The second part is the following semi-metric (symmetric) bracket representing the dissipative part defined by a symmetric transformation of the viscosity tensor

$$\prec \mathcal{F}, \mathcal{G} \succ (\varphi_t, \pi_t, \Gamma_t) = \int_{B_0} \frac{\delta \mathcal{F}}{\delta \Gamma_t} : \hat{\mathcal{V}}(\Gamma_t) : \frac{\delta \mathcal{G}}{\delta \Gamma_t}$$
(4)

This bracket structure defines the weak evolution equations $\dot{\mathcal{F}} = \{\{\mathcal{F}, \mathcal{H}\}\}\$ for all $\mathcal{F}: X \to \mathbb{R}$ with respect to a Hamiltonian $\mathcal{H}: X \to \mathbb{R}$. For this problem, the Hamiltonian is given by the sum of kinetic and total free energy:

$$\mathcal{H}(\boldsymbol{\varphi}_t, \boldsymbol{\pi}_t, \boldsymbol{\Gamma}_t) = \int_{B_0} \frac{1}{2} \boldsymbol{\rho}_0^{-1} \boldsymbol{\pi}_t \cdot \boldsymbol{\pi}_t + \Psi(\boldsymbol{C}_t, \boldsymbol{\Gamma}_t)$$
(5)

Considering the following coordinate functionals corresponding to the three state variables,

$$\mathcal{F}_{\varphi} = \int_{B_0} \delta \pi_t \cdot \varphi_t, \qquad \mathcal{F}_{\pi} = \int_{B_0} \delta \varphi_t \cdot \pi_t, \qquad \mathcal{F}_{\Gamma} = \int_{B_0} \delta \Gamma_t : \Gamma_t, \qquad (6)$$

we obtain three weak evolution equations. First, we obtain the two equations of motion given by

$$\int_{B_0} \delta \pi_t \cdot \dot{\varphi}_t = \int_{B_0} \delta \pi_t \cdot \rho_0^{-1} \pi_t, \qquad \int_{B_0} \delta \varphi_t \cdot \dot{\pi}_t = -\int_{B_0} \frac{\partial \Psi}{\partial C_t} : [\nabla \varphi_t]^T \nabla [\delta \varphi_t]$$
(7)

And second, we obtain the equation for the internal variable evolution as follows:

$$\int_{B_0} \delta \Gamma_t : \dot{\Gamma}_t = -\int_{B_0} \delta \Gamma_t : \hat{\mathcal{V}}(\Gamma_t) : \frac{\partial \Psi}{\partial \Gamma_t}$$
(8)

This set of evolution equations fulfil the following balance laws. First, we obtain total linear momentum conservation $\dot{\mathcal{P}} = \{\{\mathcal{P}, \mathcal{H}\}\} = 0$ according to the translational symmetry, where

$$\mathcal{P} = \int_{B_0} \boldsymbol{\xi} \cdot \boldsymbol{\pi}_t, \qquad \forall \boldsymbol{\xi} \in V_Q.$$
(9)

Second, a rotational symmetry of the system leads to total angular momentum conservation $\dot{\mathcal{L}} = \{\{\mathcal{L}, \mathcal{H}\}\} = 0$, where \mathcal{L} is defined by

$$\mathcal{L} = \int_{B_0} \boldsymbol{\xi} \cdot [\boldsymbol{\varphi}_t \times \boldsymbol{\pi}_t], \qquad \forall \boldsymbol{\xi} \in V_Q.$$
(10)

And third, the given brackets fulfil the balance between Hamiltonian and internal dissipation: $\dot{\mathcal{H}} = \{\mathcal{H}, \mathcal{H}\} - \prec \mathcal{H}, \mathcal{H} \succ = -\mathcal{D}_{int} \leq 0$, where the internal dissipation reads in the end

$$\mathcal{D}_{\rm int} = \int_{\mathcal{B}_0} M_t^e : \mathcal{V}^{-1} : M_t^e.$$
⁽¹¹⁾

Finite element discretisation

First, we perform a continuous spatial finite element discretisation. We approximate the spaces Q and V_Q by isoparametric finite element subspaces.

$$Q^{h} = \{ \varphi_{t}^{h} \in C^{0}(B_{0}, \mathbb{R}^{n_{\text{dim}}}) \mid \varphi_{t}^{h} = \sum_{A=1}^{n_{\text{nod}}} N_{A} x_{t}^{A} \}$$

$$V_{Q}^{h} = \{ \eta_{t}^{h} \in C^{0}(B_{0}, \mathbb{R}^{n_{\text{dim}}}) \mid \eta_{t}^{h} = \sum_{A=1}^{n_{\text{nod}}} N_{A} c_{t}^{A} \}$$
(12)

This approximation and standard arguments leads to semi-discrete evolution equations. We obtain the equation $\dot{x}_t = \mathbb{M}^{-1} p_t$ as well as the equation $\dot{p}_t = -\mathbb{Q}(C_t, \Gamma_t) x_t$ with respect to the nodal coordinate vector $x_t = (x_t^1, \dots, x_t^{n_{\text{nod}}})$ and the nodal momentum vector $p_t = (p_t^1, \dots, p_t^{n_{\text{nod}}})$. To determine the internal variable evolution, we can solve the spatial approximated weak form or the strong form at the spatial Gauss points. As in the work [4], we realise the latter and solve the equation $\dot{\Gamma}_t \Gamma_t^{-1} = 2 \left[\mathcal{V}^{-1} : M_t^e \right]$.

Now, we perform a continuous temporal finite element discretisation. For a shorter description, we combine the canonical state variables into one variable $z = (x^1, \ldots, x^{n_{\text{nod}}}, p^1, \ldots, p^{n_{\text{nod}}})$. As trial functions, we use Lagrange polynomials of degree k formulated with respect to a master element $\mathcal{T}_{\alpha} = [0,1]$, which read $z^h(\alpha) = \sum_{I=1}^{k+1} M_I(\alpha) z_I$ and $\Gamma^h(\alpha) = \sum_I M_I(\alpha) \Gamma_I$. The corresponding test functions are Lagrange polynomials of degree k - 1 given by $\delta z^h(\alpha) = \sum_{J=1}^k \tilde{M}_J(\alpha) \delta z_J$ and $\delta \Gamma^h(\alpha) = \sum_J \tilde{M}_J(\alpha) \delta \Gamma_J$. And finally, we formulate temporal weak forms of the semi-discrete evolution equations and the strong internal variable evolution:

$$\int_{0}^{1} \mathbb{J}\delta z^{h} \cdot [z^{h}]' = h_{n} \int_{0}^{1} \delta z^{h} \cdot \mathbb{H}(z^{h}) z^{h}$$

$$\int_{0}^{1} \delta \Gamma^{h} : [\Gamma^{h}]' = h_{n} \int_{0}^{1} \delta \Gamma^{h} : [2 \mathcal{V}^{-1} : M^{e}(\Gamma^{h})]\Gamma^{h}$$
(13)

Alternatively, we perform a discontinuous temporal finite element discretisation. The trial and the test functions are now Lagrange polynomials of degree *k* such that the test function now read $\delta z^h(\alpha) = \sum_{I=1}^{k+1} M_I(\alpha) \delta z_I$ and $\delta \Gamma^h(\alpha) = \sum_I M_I(\alpha) \delta \Gamma_I$. In the associated weak forms, we have therefore jump terms which enforce the initial

conditions weakly:

$$\int_{0}^{1} \mathbb{J}\delta z^{h} \cdot [z^{h}]' = \mathbb{J}\delta z_{1} \cdot [[z^{h}]] + h_{n} \int_{0}^{1} \delta z^{h} \cdot \mathbb{H}(z^{h})] z^{h}$$

$$\int_{0}^{1} \delta \Gamma^{h} : [\Gamma^{h}]' = \delta \Gamma_{1} : [[\Gamma^{h}]] + h_{n} \int_{0}^{1} \delta \Gamma^{h} : [2 \mathcal{V}^{-1}] : M^{e}(\Gamma^{h})] \Gamma^{h}$$
(14)

First, we show the natural time approximations in the constitutive laws corresponding to the cG and dG method. The trial functions directly implicate the approximation $F^h = \sum_I M_I F_I$ of the deformation gradient. The approximations C^h and $C^{e,h}$ of the strain tensors are based on the approximation of the deformation gradient. The approximations $S^{e,h}$ and $M^{e,h}$ of the 'elastic' stress tensors depend on the approximation of the 'elastic' right Cauchy-Green tensor. And the total second Piola-Kirchhoff stress tensor $S^h = 2\nabla_C \Psi^{ela}(C^h) + \mathbb{I}^{sym} : S^{e,h}[\Gamma^h]^{-t}$ then depends on the time approximation of both strain tensors.

In the eG method we apply the approach of assumed strain approximations for which we have shown in [3] that it is invariant with respect to superimposed rigid body motions. The approximation F^h of the deformation gradient has been retained unmodified from the cG method. However, the strain tensors will be now interpolated over the strains at the time nodes. Thus, we obtain the approximations $\overline{C} = \sum_I M_I C_I$ and $\overline{C^e} = \sum_I M_I C_I [\Gamma_I]^{-1}$, where $C_I = [F_I]^t F_I$. The stresses then depend on these assumed strains. The 'elastic' Mandel stress tensor is given by $\overline{M^e} = [\overline{C^e}]^t \overline{S^e}$ with the elastic stress tensor $\overline{S^e} = 2\nabla_C \Psi^{\text{ela}}(\overline{C}) + \mathbb{I}^{\text{sym}} : \overline{S^e}[\Gamma^h]^{-t}$. The main issue of the eG method, however, is its energy consistency which is based on an additionally introduced algorithmic stress tensor. We add to the approximation of the physically based stress tensor S an algorithmic stress tensor S^{alg} . The algorithmic stress tensor is a closed form expression derived from a constrained least-squares minimisation (compare in [3] the case of nonlinear elasticity). The result is the following weighted time derivative of the right Cauchy-Green tensor:

$$S^{\text{alg}} = 2 \frac{\mathcal{G}(0)}{\int_0^1 \|C'\|^2 \,\mathrm{d}\alpha]} C' \tag{15}$$

where

$$\mathcal{G}(S_{\alpha}^{\mathrm{alg}}) = \Psi_{\alpha=1} - \Psi_{\alpha=0} - \int_{0}^{1} [S_{\alpha} + S_{\alpha}^{\mathrm{alg}}] : \frac{1}{2} [C_{\alpha}]' + \frac{\partial \Psi_{\alpha}}{\partial \Gamma_{\alpha}} : [\Gamma_{\alpha}]'.$$
(16)

Numerical Example

As numerical example, we consider a general free motion of a L-shaped body initiated by an initial translation velocity vector $v_T = (6,0,0)$ and an initial an-



Figure 1: Total energy of the eG(1) (left side), cG(1) (mid position) and the dG(1) method (right side)

gular velocity vector $\omega_0 = (0, 0, 0.6)$. We used linear finite elements in time and 4-node spatial finite elements, for instance. The free energy functions are both Neo-Hookean with $\lambda = 30000$, $\mu = 7500$ and $\rho = 8.93$. The viscosities are $\eta_{dev} = 50000$ and $\eta_{vol} = 10000$.

In Figure 1, we show the total energy \mathcal{H} of the L-shaped body versus the time t computed with a medium time step size of $h_n = 0.1$. After changing time step size at t = 20, the total energy of the cG-method is increasing while the energy of the eG-method continued to decrease. A further disadvantage of the cG-method is the only time-averaged decrease using this medium time step size. Using the numerically dissipative dG-method for computing this motion, the total energy also decreases. However, after changing time step size, we obtain a jump in the total energy and a further decrease in the equilibrium state.

Reference

- 1. Argyris J.H. and Scharpf D.W. Finite elements in time and space, Nucl. Engrg. Design 10 (1969) 456-464.
- Betsch P. and Steinmann P. Inherently Energy Conserving Time Finite Elements for Classical Mechanics, Journal of Computational Physics 160 (2000) 88-116.
- Groß M., Betsch P. and Steinmann P. Conservation properties of a time FE method-part IV: Higher order energy and momentum conserving schemes, Int. J. Numer. Meth. Engng. 63 (2005), 1849-1897.
- 4. Reese S. and Govindjee S. A Theory of Finite Viscoelasticity And Numerical Aspects, Int. J. Solids Structures 35 (1998), 3455-3482.