Higher-order accurate and energy-momentum consistent discretisation of dynamic finite deformation thermo-viscoelasticity

dem Fachbereich Maschinenbau

der Universität Siegen

zur Erlangung der venia legendi für das Fach

MECHANIK

vorgelegte Habilitationsschrift

von

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eingereicht am

8. Oktober 2008

Habilitationsverfahren vollzogen am

26. Juni 2009

ZUSAMMENFASSUNG

Diese Arbeit behandelt die energiekonsistente Simulation von Bewegungen eines viskoelastischen kontinuierlichen Körpers, unter Einbezug der Kopplung von thermischen und mechanischen Feldern. Der verwendete Algorithmus basiert auf einer Vier-Feld-Formulierung in Lagrangescher Darstellung, in der die Deformationsabbildung, das Geschwindigkeitsfeld, das Temperaturfeld und eine deformationswertige viskose innere Variable unabhängige Variablen darstellen. Die Bewegungsgleichungen sind deshalb Differentialgleichungen erster Ordnung. Das Lagrangesche Temperaturfeld wird bestimmt durch die lokale Entropiebilanz als dritte Differentialgleichung erster Ordnung, verbunden mit dem Fourierschen Gesetz für Wärmeleitung. Die letzte Differentialgleichung erster Ordnung stellt die viskose Evolutionsgleichung dar. Sie basiert auf einer inneren Dissipation, welche quadratisch in einem nichtlinearen viskosen Verzerrungsratentensor formuliert ist.

Dieses System von gekoppelten nichtlinearen Differentialgleichungen wird diskretisiert mittels einer neuen Raum-Zeit-Finite-Elemente-Methode, die sowohl zu kontinuierlichen als auch zu diskontinuierlichen Approximationen in der Zeit führt. Aufgrund spezieller Zeitapproximationen in den konstitutiven Gesetzen des Problems wird, neben der Gesamtimpuls- und Gesamtdrehimpulsbilanz, auch eine Stabilitätsabschätzung bezüglich einer relativen Energiefunktion noch nach der Raum-Zeit-Diskretisierung exakt erfüllt. Daher ist der resultierende Zeitintegrationsalgorithmus langzeitstabil, auch wenn Zeitschrittweitenänderungen vorgenommen werden.

Das erhaltene System von gekoppelten nichtlinearen algebraischen Gleichungen wird mittels einer monolithischen Strategie gelöst. Die damit verbundenen Newton-Raphson-Verfahren auf globaler Ebene und auf Elementebene basieren auf einer konsistenten Linearisierung. Die verwendeten neuen Konvergenzkriterien für die iterative Lösungsprozedur beziehen die Energiekonsistenz des Algorithmus' in Betracht, und sind frei von Skalierungseinflüssen in den vier unabhängigen Variablen. Repräsentative numerische Simulationen mit verschiedenen Randbedingungen zeigen die unbegrenzte Genauigkeit und die hervorragende Stabilität des neuen Zeitintegrationsalgorithmus'.

Schlagwörter: Multi-physikalische Problemstellungen, Starke thermomechanische Kopplung, Raum-Zeit-Finite-Elemente-Methode, Zeitschrittverfahren, Energie-Impuls-Konsistenz, Höhere Genauigkeitsordnung, Monolithische Lösungsstrategie, Konsistente Linearisierung, Skalierungsfreie Konvergenzkriterien.

ABSTRACT

This paper is concerned with the energy consistent simulation of motions of a viscoelastic continuum body, under inclusion of the coupling of thermal and mechanical fields. The corresponding algorithm is based on a four-field formulation in the Lagrangian description, in which the deformation mapping, the velocity field, the temperature field and a strain-like viscous internal variable field are independent unknowns. Hence, the equations of motion are formulated in first-order form. The Lagrangian temperature field is determined by the first-order entropy evolution equation, associated with Fourier's law of heat conduction. The first-order viscous evolution equation is derived from an internal dissipation being quadratic in a nonlinear viscous strain-rate tensor.

This coupled system of nonlinear differential equations is discretised by a new space-time finite element method, consisting of continuous as well as discontinuous finite element approximations in time. Owing to particular time approximations in the constitutive laws, beside the total linear momentum as well as the total angular momentum balance, a nonlinear stability estimate with respect to a relative energy function is exactly fulfilled in the fully discrete case as well. Hence, the resulting time integration algorithm is long-time nonlinear stable also when changing the time step size.

The obtained coupled system of nonlinear algebraic equations is solved by a monolithic solution strategy. The corresponding Newton-Raphson methods on the global and the element level are based on a consistent linearisation. The new convergence criteria used for these iterative solution procedures take the energy consistency into account, and is free of the scaling in the independent variables. Representative numerical simulations with various boundary conditions show the higher-order accuracy and the superior stability of the new time integration algorithm.

KEYWORDS: Multi-Physics Problems, Strong Thermo-Mechanical Coupling, Space-Time Finite Element Methods, Time-Stepping Algorithms, Energy-Momentum Consistency, Higher-Order Accuracy, Monolithic Solution Strategy, Consistent Linearisation, Scaling-Free Convergence Criteria.

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1. INTRODUCTION

In the dynamic finite deformation elasticity, it turned out that well-known stability estimates for linear problems are not valid for nonlinear problems. First statements about this topic can be found in Belytschko & Schoeberle [1] and Hughes [2]. On the other hand, representative numerical simulations reveal that time integration algorithms can possess instable behaviour (see Simo & Tarnow [3] and Crisfield & Shi [4], for instance). This numerical instability is identifiable through the divergence of the used iterative solution procedure, induced by unphysical time evolutions. In Crisfield & Shi [4], this behaviour is designated as locking in time, in the light of the well-known locking in space occurring in calculations with shells and quasi-incompressible material. In order to avoid the temporal locking with elastic material, two common approaches are the development of conserving, in particular energy conserving, time integration algorithms, or the introduction of numerical dissipation by the time integrator for damping out high-frequent modes.

The approach of energy conserving time integration algorithms is based on the fact that energy conservation means unconditional numerical stability (see Richtmyer & Morton [5] and Wood [6]). This knowledge is confirmed several times during the numerical time integration of conservative systems, especially of hyperelastic systems. For instance, the authors of LaBudde & Greenspan [7, 8] investigated energy conserving time integration algorithms for N-body problems. By considering Hamiltonian systems in Simo et al. [9], the meaning of total linear as well as total angular momentum conservation for the numerical time integration is realised. In Simo & Tarnow [3], this approach is applied to dynamic finite deformation elasticity, and leads to energy-momentum conserving time integration algorithms. Here, the stability of an exact energy conserving time integration is confirmed again. This algorithm is based on a midpoint approximation together with modified internal forces. In Gonzalez [10], the time integration algorithm is also composed of these two elements. However, the latter algorithm arise from the well-known approach of substituting a discrete derivative for an analytical derivative in the discretisation. The discrete derivative approach is already applied to the N-body problem in Greenspan [11, 12]. The origin of this approach is the view

of a conserving time integration algorithm as discrete conservative mechanical system, or discrete Hamiltonian system, respectively (see Greenspan [13]). From this perspective, the positive influence of exact algorithmic conservation properties on numerical stability and physical quality of the numerical solution is analytically proved for a model problem in Gonzalez & Simo [14]. Unlike a discrete stress tensor, a temporal continuous energy conserving stress approximation is presented in Sansour et al. [15]. In this reference, the energy-momentum conserving time integration algorithm for shells is based on a covariant continuum formulation. In Groß et al. [16], a temporal continuous and energy-momentum conserving stress approximation is given as well. However, this approach includes the effective discrete gradient in Gonzalez [10] in the case of a midpoint approximation. An alternative to modifying internal forces is to enforce the exact energy conservation iteratively as constraint by means of a Lagrange multiplier. The authors of Hughes et al. [17] apply this concept on the basis of the trapezoidal rule. In Laursen & Meng [18], exact energy conservation is also achieved iteratively, using the energy conservation condition as additional equation for determining a scalar-valued parameter field. Energy-momentum conserving time integration algorithms for nonlinear structural dynamic problems are constructed in Simo & Tarnow [19] and Simo et al. [20]. A similar proceeding in Crisfield & Shi [4, 21] leads to an energy-momentum conserving time integrator for trusses, in Galvanetto & Crisfield [22] for two-dimensional beams, and in Zhong & Crisfield [23] for shells. The authors of Stander & Stein [24] also present a conserving time integrator for two-dimensional beams, and Brank [25] deals with the extension of the conserving time integrator for dynamic shell motions in the foregoing Reference Brank et al. [26] to flexible laminates. In connection with an iterative enforcement of the energy conservation in structural dynamics, we mention Kuhl & Ramm [27], wherein, in addition to the total energy conservation, also the total linear and total angular momentum conservation is enforced by Lagrange multipliers. Unusually, the time approximation is based on a numerically dissipative time integration algorithm. Hence, high-frequent modes of the solution are damped out, however, the decrease of total energy owing to the numerical dissipation is balanced by the energy conservation constraint.

The approach of introducing numerical dissipation by means of a time integrator arise from the knowledge about linear stability of time integration algorithms. Since the maximum time step size of linear stable time integration

algorithms is inversely proportional to the highest frequency of the discrete system, the approach of damping out high-frequent modes of the solution in order to increase the time step size stand to reason (see Hilber et al. [28]). Assumption is that these modes are not of primary interest for the considered motion. The locking effect in time of nonlinear problems, mentioned in Crisfield & Shi [4], is also traced back to high-frequent modes. In the dynamic finite deformation elasticity, this approach is applied, because a finite element approximation in space does not approximate high-frequent modes very well (see Strang & Fix [29]). Therefore, numerically dissipative time integration algorithms are developed for nonlinear elastic materials (compare Armero & Romero [30, 31] for elastic continuum elements and Ibrahimbegovic & Mamouri [32] for elastic beam elements). However, in the knowledge of the present authors, it is not sufficiently clear in the scope of nonlinear problems, if numerically dissipative time integration algorithms do not also damp out physically relevant modes of the solution. Therefore, this approach is not considered in the present work.

The aforementioned references show that the exact fulfilment of energy and momentum balances is an important quality feature of time integration algorithms for nonlinear elastodynamics. However, the therein presented time integrators are at most second order accurate. A more accurate solution can only be achieved by a smaller time step size. This, however, can be numerically more costly. For this reason, the approaches behind the energy-momentum conserving time integration algorithms in Gonzalez [10, 33] and Simo & Gonzalez [34] are carried forward into higher-order accurate time integration schemes in Groß et al. [16] and Groß [35]. These time integrators show the stability properties for arbitrary accuracy orders. The improved numerical stability allows to use larger time steps, and leads to more efficient calculations. The approach is based on the Galerkin method, which allows a systematical construction of implicit time integration algorithms of arbitrary accuracy order by means of finite elements in time. Temporal Galerkin methods are mainly subdivided into discontinuous Galerkin (dG) methods and continuous Galerkin (cG) methods (see Eriksson et al. [36]).

In dG methods, the approximation of the test function and the trial function is assumed to be discontinuous over the element boundaries. The dG method is traced back at least to Lasaint & Raviart [37], and is described in detail in Cockburn [38] and Thomee [39], for instance. A first application on linear elastodynamics is given in Hughes & Hulbert [40], wherein

simultaneously a Galerkin method in space is applied. In Hulbert [41, 42], it is focused on the numerical treatment of the semi-discrete equations. Thereby, the authors decide between a single-field formulation and a two-field formulation. In the former formulation, one uses only trial functions in the displacements, where in the latter formulation, one also applies independent trial functions for the velocities. For example, in Li & Wiberg [43, 44], the dG method is implemented with linear finite elements in time for the displacements as well as for the velocities. This work is extended to a nonlinear model problem in Wiberg & Li [45]. Likewise, nonlinear model problems are considered in Bonelli & Bursi [46] and Bottasso [47]. The former reference elaborates on the connection between dG and Runge-Kutta methods. In the latter reference, the dG method is applied to stiff differential equation systems, and the numerical cost is compared. The application of the dG method to nonlinear beams is subject of Bauchau & Theron [48]. This formulation is extended to elastic multibody systems in Bauchau & Bottasso [49]. However, when applied to hyperbolic problems as the nonlinear elastodynamics, the dG methods lead to time integration algorithms with numerical dissipation. Using constant finite elements in time, for instance, we obtain the well-known implicit Euler method. Therefore, the dG method is a way of introducing numerical dissipation, and belongs to the second approach for obtaining stable time integration algorithms. For this reason, the time integration algorithms for the nonlinear problems in Bauchau & Bottasso [49] and Bauchau & Theron [48] is based on the dG method. In Groß et al. [50] and Groß [51], however, is shown that the ordinary dG method is not appropriate to construct momentum conserving time integration algorithms, owing to the jump in the time evolution. Only a reduced time integration in the resulting finite element method leads to total angular momentum conservation. This integration, with less Gauss points as in fact for the used polynomial degree of the shape functions is necessary, is already known from the volume integration in specific continuum elements. For example, it is used to avoid locking of continuum elements for quasi-incompressible material (see Wriggers [52] for an overview). On the other hand, the reduced time integration in the dG method leads to a time integration algorithm being identical to that, which follows by a consistent time integration from an ordinary cG method. For this reason, the authors of Groß et al. [50] and Groß [51] apply only the cG method for designing conserving time integrators of arbitrary order. Note that independent of the results in Groß [51], the authors of Larson & Niklasson [53]

have shown that the cG method can be viewed as a limit of the dG method if a parameter tends to infinity.

In cG methods, the approximation of the trial functions is assumed to be continuous over the element boundaries, whereas the approximation of the test functions is further discontinuous. Therefore, we obtain implicit time integration algorithms. The cG method seems to go back to Douglas & Dupont [54] and Swartz & Wendroff [55] for parabolic problems, and to Hulme [56, 57] for ordinary differential equations. More details about the continuous Galerkin method can be found in Eriksson et al. [36] and Fairweather [58], for instance. In Aziz & Monk [59] and Winther [60], the cG method is also applied to solve partial differential equations. In French & Schaeffer [61], the time integration of ordinary and different nonlinear partial differential equations is investigated. In this reference, the aspect of exact energy conservation is also treated, and leads to an energy conserving time integration algorithm. In a follow up paper, the exact energy conservation is also considered as important for nonlinear wave propagation (see French & Peterson [62]). That the cG method is particulary appropriate to construct energy conserving time integration algorithms for conservative problems is also found by other authors. For example, in Betsch & Steinmann [63] is shown that just the cG method is inherently energy conserving, which means the energy conservation is achieved for exact calculation of time integrals. This property leads to a better and better conserved energy with increasing accuracy order of the numerical quadrature. Also in Larson & Niklasson [64], the conservation properties of the cG method is investigated and compared with that of the dG method. In Betsch & Steinmann [65], an energy-momentum conserving time integration is designed for the N-body problem. This formulation is extended to semidiscrete nonlinear elastodynamics in a follow up paper (see Betsch & Steinmann [66]). Since the exact energy-momentum conserving time integration algorithms in these works are at most second order accurate, the part Groß et al. [16] of this publication series shows the extension to higher-order accurate energy-momentum conserving time integration of both problem classes. The third part also describes the conserving time integration of coupled elastic and rigid bodies with second-order accurate integrators (see Betsch & Steinmann [67]).

In the present work, we also apply the Galerkin method in time combined with a Galerkin method in space. In this way, we obtain a space-time approximation, which is not restricted in the accuracy order. Whether we

use a cG or dG method in time is based upon the consistency with energy balances of our now dissipative problem.

1.1. Literature review

In all of the mentioned references about energy conserving time integrators for nonlinear elastodynamics is found that an indicator for an unstable numerical integration is the so-called blow-up behaviour. This phenomenon means a steadily increased total energy with increasing calculation duration. An energy blow-up is noticed particularly with high material stiffness. If no blow-up behaviour is observed, the energy oscillates around a constant energy level. Consequently, energy inconsistent non-dissipative algorithms produce algorithmic energy during the integration of elastic systems. In dynamic problems of dissipative materials is expected that this algorithmically produced energy is compensated if the physical dissipation is sufficiently high. And so, the numerical instability cannot be observed. This compensation is observed in Simo [68], during the time integration of motions of plastic materials. In the same reference, a non-conserving time integration algorithm is compared with a total linear and total angular momentum conserving algorithm. By using numerical simulations, the author concludes that the latter is more stable than the non-conserving time integrator. Hence, the relevance of momentum conserving time integration algorithms is verified also for dissipative materials.

This expected compensation of algorithmically produced energy is not observed in each case. In Meng & Laursen [69], it is described that a not sufficiently high internal dissipation of a plastic material leads to an energy blow-up with subsequent numerical instability. However, this blow-up behaviour is avoided by using an energy consistent time integration algorithm, which is an algorithm fulfilling exactly the discrete energy balance. In the conservative case, the energy is conserved, and in the dissipative case, the approximated physical dissipation leads to a prescribed energy loss. In this paper, algorithms for the additive as well as multiplicative plasticity with isotropic hardening are presented. In Noels et al. [70], a variational formulation with incremental potentials according to Ortiz & Stainier [71] allows the construction of a conserving time integrator for elastoplasticity, which is based on the discrete derivative approach for hyperelastic materials according to Gonzalez [10]. The procedure in Noels et al. [70] is not restricted to isotropic