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Algorithms for coupled problems that preserve symmetries and the laws of thermodynamics
Part II: fractional step methods

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ABSTRACT

This article proposes a new type of discretizations for initial boundary value problems of thermodynamical systems. Based on a combination of finite elements in space and fractional step methods in time, we formulate algorithms that exactly preserve the symmetries and the laws of thermodynamics of the continuum problem. The algorithmic design is based on the GENERIC formalism of irreversible thermodynamics which naturally suggests the split of the evolution operator upon which our fractional step method is based. Although the emphasis of the article is on the generality of the results, as an illustration, a discretization of nonlinear, finite strain, thermoelasticity is presented. Numerical simulations are provided that verify the excellent performance of the new methods.

1. Introduction

Applied mathematicians and mechanicians continue to search for better discretization methods for approximating the solution of the evolution problems that commonly appear in problems of fluid, solid, structural, and celestial mechanics, thermodynamics, molecular dynamics, and many other disciplines. Broadly speaking, the goals of such efforts are to formulate numerical methods with increased accuracy, robustness, and which replicate in the discrete setting the most important features of the continuum problem, hence providing insight into the physics of the real problem.

The last goal has motivated the development of structure preserving algorithms (see, for example, the monographs [1–4]). This diverse family of methods, also known as geometric integrators, is designed to produce numerical solutions that inherit some of the most important qualitative properties of the systems they approximate. For instance, integrators for Hamiltonian evolution equations aim to preserve the symplectic structure [5], the Lagrangian structure [6,7], or energy and momenta [8–12]. For this class of problems, in particular, the rich geometric structure of the continuum equations has guided the numerical developments. For other type of problems, the lack of a unifying mathematical structure has hindered the development of general purpose, structure preserving discretizations.

In [13], henceforth referred to as Part I, we presented a framework for the design of discretizations that, when applied to the evolution equations of general thermodynamical systems, preserve the two laws of thermodynamics as well as the possible symmetries. The range of problems to which this new approach can be applied is very wide, including in particular Hamiltonian mechanics. In the latter case, the proposed algorithms reduce to the Energy–Momentum method as described in [10,14]. The new methods are thermodynamically consistent because when applied to isolated thermomechanical systems, yield approximations whose energy remains strictly constant and its entropy never decreases. Furthermore, when the evolution equations have symmetries, the algorithms preserve them as well.

The theoretical background for the new thermodynamically consistent methods, TC methods hereafter, is the GENERIC (General Equations for Non-Equilibrium Reversible–Irreversible Coupling) formalism for non-equilibrium thermodynamics as developed originally in [15] and summarized in the monograph [16,17]. This framework generalizes Hamiltonian mechanics to dissipative systems and sets up an abstract formulation that separates the reversible and irreversible parts of the evolution operator. To discretize the reversible dynamics, the TC methods employ the ideas of the Energy–Momentum methods. For the irreversible part, a novel discretization technique is employed which preserves the dissipative character without any coupling with the reversible terms. Respecting this decoupling in the discrete setting is crucial for the formulation of algorithms that mimic the thermodynamic structure of the continuum problems.

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In Part I we proposed TC algorithms for general, infinite dimensional, thermomechanical problems. The spatial discretization is based on finite elements and the integration in time employs a modified midpoint rule, resulting in monolithic schemes. As an application, we showed the solution obtained with the new methods to the problem of finite strain thermoelasticity, illustrating the conservation properties as well as the remarkable robustness of the method in representative simulations. The most important drawback of such methods is the computational cost associated with the coupled solution of all the thermodynamic variables at all the nodes of the finite element mesh. To improve this situation, we propose in the current article TC staggered algorithms with the same properties as the monolithic ones, but with less CPU cost.

The basic idea of the methods proposed in this article is to continue exploiting the GENERIC split of the evolution equations in coupled problems. By using a TC method for the reversible part of the flow (which is identical to an Energy–Momentum algorithm) and another TC method for the irreversible part, fractional step methods with the desired conservation properties can be obtained. The resulting methods share the qualitative correctness of their monolithic counterparts but are substantially faster. Moreover, not only the full integrator is thermodynamically consistent, but also each one of the fractional steps. In the same way that energy conservation/entropy dissipation has a positive effect on the robustness of the monolithic TC algorithms, the proposed staggered methods are remarkably robust. These ideas were earlier explored by the author in [18] for evolution problems in finite dimensional spaces and are given full generality in the current article.

The landmark work on fractional step methods by Armero and Simo [19–22] has similarities with the proposed algorithms. These authors showed that by a judicious choice of the operator split in the continuous equations of an evolution problem, important stability improvements can be gained in fractional step methods derived from them. Furthermore, it was shown that this increase in the numerical robustness was ultimately due to the fact that each one of the (partial) evolution operators of the split preserved the stability of the complete problem. The work in the current article improves these results in two ways: first, the appropriate split for the evolution equations need not be guessed anymore because it is dictated by the GENERIC evolution equation; second, the stability estimate of the evolution problem is not only inherited by each one of the partial evolution operators, but also by the discrete time marching schemes, in each of the fractional steps. This latter property results in even further robustness of the numerical solution.

As an application of the proposed methods, we consider as in Part I finite strain thermoelasticity. The derivation of the update equations for the staggered TC methods is worked out in detail. Numerical examples are presented which illustrate the conservation properties as well as the robustness of the method as compared with other standard fractional step methods.

A summary of the rest of the article is as follows. Section 2 reviews the essential features of GENERIC. In Section 3 we review the TC monolithic algorithms introduced in Part I. These two sections provide the continuum and discrete background for the development of a new class of fractional step methods, as described in abstract form in Section 4. An application of the general methodology is given in Section 5, where the full discretization of the finite strain thermoelasticity in the context of the new methods is described in detail. Numerical results of the resulting formulations are given in Section 6, where the proposed methods are compared with existing staggered schemes. The article concludes with a summary of results in Section 7.

2. Evolution equations in GENERIC

At the core of the algorithms discussed in this article is GENERIC, a recently proposed formalism that tries to unify the mathematical description of non-equilibrium thermodynamics by providing a common structure to their evolution equations. This framework is fully developed in [16] and has been summarized in Part I. In this section we provide the essential ingredients of GENERIC for infinite dimensional systems, introducing the notation for the rest of the article.

2.1. Basic definitions

We consider thermomechanical systems consisting of a deformable body $\mathcal{B}_o \subset \mathbb{R}^n$ with points denoted $\boldsymbol{X}$ and thermodynamic state space $\mathcal{S}$, which includes all smooth mappings $z:\mathcal{B}_o \to \mathbb{R}^m$. The set $\mathcal{S}$ is assumed to be a subset of an infinite dimensional vector space $\mathcal{V}$ with inner product $\langle \cdot,\cdot \rangle: \mathcal{V}\times\mathcal{V}\to\mathbb{R}$ and which we identify with its dual $\mathcal{V}^*$. The tangent space of $\mathcal{S}$ can be identified with $\mathcal{V}$ itself. The functional derivative of a functional $\mathcal{F}:\mathcal{S}\to\mathbb{R}$ is denoted $\dfrac{\delta \mathcal{F}}{\delta z}$.

For the mathematical description of the evolution problems of interest two types of bilinear operations are required. First, a Poisson bracket is an operation mapping two functionals $\mathcal{F}$, $\mathcal{G}$: $\mathcal{S}\to\mathbb{R}$ into a new functional $\{\mathcal{F}, \mathcal{G}\}$: $\mathcal{S}\to\mathbb{R}$. The operation $\{\cdot,\cdot\}$ must be bilinear, skew-symmetric, and satisfy Leibniz and Jacobi properties. Second, a dissipative bracket is defined to be another bilinear operation taking two functionals $\mathcal{F}, \mathcal{G}$ as above, into a new functional $[\mathcal{F}, \mathcal{G}]$: $\mathcal{S}\to\mathbb{R}$. This second operation must be symmetric and positive semidefinite.

Associated with the previous brackets, there exist differential operators $\boldsymbol{L}$, $\boldsymbol{M}$: $\mathcal{S}\times\mathcal{V}\to\mathcal{V}$ defined by the relations:

$$\{\mathcal{F},\mathcal{G}\} = \left\langle \frac{\delta \mathcal{F}}{\delta z}, L(z)\left[\frac{\delta \mathcal{G}}{\delta z}\right]\right\rangle \quad , \quad [\mathcal{F},\mathcal{G}] = \left\langle \frac{\delta \mathcal{F}}{\delta z}, M(z)\left[\frac{\delta \mathcal{G}}{\delta z}\right]\right\rangle. \tag{1}$$

For any pair $(z, \boldsymbol{V})\in\mathcal{S}\times\mathcal{V}$ we write $\boldsymbol{L}(z)[\boldsymbol{V}]$ instead of $\boldsymbol{L}(z, \boldsymbol{V})$ to stress that the operator $\boldsymbol{L}$ must be linear on its second argument. Often, the explicit dependence of $\boldsymbol{L}$ on the state variable z is omitted. The same convention applies to the friction operator $\boldsymbol{M}$.

2.2. The GENERIC evolution equations

Next we consider isolated thermomechanical systems with total energy E and entropy S, respectively. If its thermodynamic state in time is described by a curve $z_t:[0, T]\to\mathcal{S}$ then the GENERIC equations of evolution can be written as

$$\dot{\mathcal{F}}(z_t) = \{\mathcal{F}(z_t), E(z_t)\} + [\mathcal{F}(z_t), S(z_t)], \tag{2}$$

for any functional $\mathcal{F}:\mathcal{S}\to\mathbb{R}$. In the previous equation the superposed dot indicates the time derivative.

Whereas the specific form of the brackets is not known for all thermodynamical systems, the GENERIC formalism guarantees that if found, the evolution equations (2) model the dynamics of a system that strictly satisfies the two laws of thermodynamics as long as the brackets satisfy the degeneracy conditions:

$$\{S,\mathcal{F}\} = [E,\mathcal{F}] = 0, \tag{3}$$

for every functional $\mathcal{F}:\mathcal{S}\to\mathbb{R}$. In terms of the operators $\boldsymbol{L}$ and $\boldsymbol{M}$, the degeneracy conditions read:

$$\left\langle \frac{\delta \mathcal{F}}{\delta z}, L\left[\frac{\delta S}{\delta z}\right]\right\rangle = \left\langle \frac{\delta \mathcal{F}}{\delta z}, M\left[\frac{\delta E}{\delta z}\right]\right\rangle = 0. \tag{4}$$

For the numerical implementation of the GENERIC equations of evolution it proves useful to write (2) in weak form. To that end, we define the vector field $w = \frac{\delta \mathcal{F}}{\delta z}$, use the definition of directional derivative and the operators (1) to rewrite the GENERIC evolution equations as:

$$\langle w, \dot{z}_t\rangle = \left\langle w, L\left[\frac{\delta E}{\delta z}\right]\right\rangle + \left\langle w, M\left[\frac{\delta S}{\delta z}\right]\right\rangle. \tag{5}$$