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Variational space–time elements for large-scale systems

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Abstract

In this paper, we introduce a new Galerkin based formulation for transient continuum problems, governed by partial differential equations in space and time. Therefore, we aim at a direct finite element discretization of the space–time, suitable for massive parallel analysis of the arising large-scale problem. The proposed formulation is applied to thermal, mechanical and fluid systems, as well as to a Kuramoto–Sivashinsky problem, representing the general class of higher-order formulations in material science using NURBS based shape functions. We verify whenever possible the conservation properties of the formulation. Finally, a series of examples demonstrate the applicability to all systems presented in this paper.

Keywords: Space–time; Large-scale; Galerkin; IGA; Parallel; Multigrid

1. Introduction

The most important mathematical framework for the numerical analysis of partial differential equations (PDEs) has been developed by Galerkin using a weak form on a Hilbert space. On this basis, Courant formulated in 1943 a variational method for the solution of Galerkin type problems [1]. This leads to the first application of finite elements in 1956 by Turner et al. [2]. Driven by statical problems in engineering, finite element solutions of spatial systems have been further improved (see, among many others, Zienkiewicz et al. [3] and Belytschko et al. [4,5]) and higher continuity basis functions like B-Splines in the context of Isogeometric Analysis (IGA) was introduced by Hughes et al. [6]. Further extensions have been proposed throughout the past two decades for the calculation of multi-physical phenomena, e.g. thermomechanical Systems (see, among many other, Simo & Holzapfel [7], Hesch & Betsch [8]), fluid systems (see Donea & Huerta [9]), material science (see e.g. Anders et al. [10]) and many other formulations.

The fundament remains: variational formulations in space are widely used in structural mechanics, whereas in the temporal regime, both, weak and strong forms have been proposed, see Hughes et al. [11,12] for an example of a classical time stepping method. First applications on finite elements in time can be traced back to Bailey [13],

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dealing with the transient behaviour of beams. Further developments can be found in Gellin & Pitarresi [14], Pitarresi & Manolis [15] and Atilgan et al. [16], see also Bottasso [17]. Space–time finite element methods have also been considered in fluid dynamics, see Hughes and Hulbert [18], Hughes et al. [19] and Shakib and Hughes [20], for two-phase flow in [21], see also Betsch et al. [22–24] for a series on finite element formulations in time. In the majority of finite element formulations in time, the semidiscrete equations are, however, multiplied by weighting functions in space and time and integrated over time. As already shown in Hughes & Hulbert [18], *this negates one of the most powerful features of the finite element method: unstructured meshes*. More importantly, it restricts adaptive methodologies either to space only or/and to global refinement in time.

Due to restricted computational capacities, and above all due to our own personal experience, all methods have been designed to march forward in time. Even the above mentioned finite element formulations in time have been formulated using a Petrov–Galerkin method with different shape function of the functional solution and test spaces to obtain a time-discontinuous Galerkin formalism. This approach leads to a lower triangular matrix for the total system to be solved in space and time and ensures that information flows always in the direction of positive time, i.e. solutions are said to be *causal* since they depend upon the past but not on the future. And although this is natural in our human perspective, it certainly may not be optimal from a computational point of view. We note, however, that the first time-parallel approach for ordinary differential equations was already presented more than 50 years ago in [25].

As a remedy, we propose a Bubnov–Galerkin approach using continuous finite elements in time and space–time, i.e. we apply the same shape functions for the solution as well as for the test functional space. This approach can be derived in a variationally consistent way, hence we can demonstrate all necessary conservation properties of the different systems under consideration. The application of domain-decomposition methods is formally straight forward, we only have to consider to work in the $\mathbb{R}^{n+1}$ dimensional space–time. For two-dimensional problems in space, existing solvers for three-dimensional problems can be applied directly to solve the arising, massive large-scale problem. However, certain modifications might be necessary as the differential operator in time behaves differently than in space.

Multigrid methods, which have been developed since the 50s of the last century, allow for the solution of sparse symmetric positive definite linear system with optimal complexity, cf. [26]. Thanks to their optimality and also their parallel scalability, multigrid methods have turned into a standard choice for the solution of large scale systems arising from the discretization of elliptic PDEs. During the last decades, extensions of multigrid have been developed which have also shown to be efficient and robust also in non-linear systems, such as frictional non-linear elasticity, and saddle-point problems. Multigrid methods have also been successfully applied to the linear systems arising from the full space–time discretization of parabolic systems, see, e.g. [27,28]. The fact that for parabolic equations, the differential operator in time direction is only of first order and not of second order, as it is in space, requires some modifications of the multigrid method. These modifications are realized usually by special choices of the smoother, i.e. line smoothers, or by special coarsening strategies. In particular the modifications of the smoother are related to smoothing strategies which have been proposed for convection-dominated elliptic problems, such as convection–diffusion. Another possibility is to introduce on the discrete level mesh-dependent diffusion in time, cf. [29]. For general non-linear problems, multigrid methods for non-linear problems can be employed, leading to the PFASST-method (Parallel Full Approximation Scheme in Space and Time), see [30]. Again, the treatment of the time-direction within a multi-level scheme requires particular care, cf., e.g. [31].

In general, for the discretization in time direction for space–time multigrid methods, in the literature the following approaches can be identified:

- to use discontinuous Galerkin in time. This approach is the most widely used, see e.g. [28,29,32], based on the formulation originally presented in [33].
- to use tailored test functions, containing a time-derivative of the space–time continuous test functions. This means to replace a standard test function $\delta\theta$ with $\delta\theta \Rightarrow \nabla_t \delta\theta$, or to add this expression to the otherwise unchanged test-function. This formalism has been presented in [34] and has been shown to be equivalent to a Petrov–Galerkin formulation
- to use continuous ansatz-spaces in space and time, see, e.g. [35] and [36]. We note that these works are dealing with the wave equation, where time and space derivatives are of the same order.

Space–time multigrid for parabolic problems, using finite differences and a Gauß–Seidel smoother have been used in [37]. Interestingly, if only coarsening in space is applied, standard multigrid performance is achieved. If coarsening