



Variational time discretization for mixed finite element approximations of nonstationary diffusion problems



Markus Bause*, Uwe Köcher

Helmut Schmidt University, University of the Federal Armed Forces Hamburg, Department of Mechanical Engineering, Holstenhofweg 85, 22043 Hamburg, Germany

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ABSTRACT

We develop and study numerically two families of variational time discretization schemes for mixed finite element approximations applied to nonstationary diffusion problems. Continuous and discontinuous approximations of the time variable are encountered. The solution of the arising algebraic block system of equations by a Schur complement technique is described and an efficient preconditioner for the iterative solution process is constructed. The expected higher order rates of convergence are demonstrated in numerical experiments. Moreover, superconvergence properties are verified. Further, the efficiency and stability of the approaches are illustrated for a more sophisticated three-dimensional application of practical interest with discontinuous and anisotropic material properties.

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1. Introduction

Numerical simulations of time dependent single and multiphase phase flow and multicomponent transport processes in porous media are desirable in several fields of natural sciences and in a large number of branches of technology; cf. e.g. [1]. The categories are far from clear-cut, but include environmental engineering (groundwater and soil contamination), hydrology, geophysics, agricultural, sanitary and chemical engineering, metal casting, ceramic engineering as well as petroleum engineering, geothermal energy recovery, carbon (dioxide) capture and storage in geological structures, gas injection as an efficient method of enhanced oil recovery and the technologies of wood, paper, cement, lightweight composite materials (aerospace engineering) and pharmaceuticals. Further, temperature changes may accompany the physical and chemical processes. Temperature variation then influences the multiphase flow and multicomponent transport by altering physical and chemical properties of the phases such as densities, viscosities and reaction rates.

The accurate numerical approximation of such flow and transport processes in heterogeneous and anisotropic porous media continues to be a challenging task. As a prototype model system we may consider the nonlinear set of coupled partial differential equations

$$\partial_t(\Theta c_l) + \nabla \cdot (\mathbf{D}_l \nabla c_l - \mathbf{Q} c_l) = R_l(c_1, \dots, c_L) \quad \text{in } \Omega \times I, \quad (1.1)$$

$$c_l = g_{D,l} \quad \text{on } \Gamma_D \times I, \quad (1.2)$$

$$-(\mathbf{D}_l \nabla c_l - \mathbf{Q} c_l) \cdot \mathbf{n} = g_{F,i} \quad \text{on } \Gamma_F \times I, \quad (1.3)$$

$$c_l(\cdot, 0) = c_l^0 \quad \text{in } \Omega \times \{0\} \quad (1.4)$$

* Corresponding author.

E-mail address: bause@hsu-hh.de (M. Bause).

URL: <http://www.hsu-hh.de/mb-mathe> (M. Bause).

for $l = 1, \dots, L$, with $L \in \mathbb{N}$. Eq. (1.1) includes the effects of advective, diffusive and reactive transport in a multicomponent system with the unknown vector $\mathbf{c} = (c_1, \dots, c_L)^\top$ of concentrations of mobile chemical species. In (1.1)–(1.4), we denote by $I = (0, T)$ a finite time interval and $\Omega \subset \mathbb{R}^d$, with $d = 2$ or $d = 3$, is a domain with Lipschitz-continuous boundary Γ which is split into a flux boundary Γ_F and a Dirichlet boundary Γ_D . The outer unit normal vector to Ω is denoted by $\mathbf{n}$. The rates $R_i(c_1, \dots, c_L)$ model chemical reaction rates and sources and sinks. Further, Θ denotes the volumetric water content, $\mathbf{Q}$ the Darcy flux and $\mathbf{D}_l \in \mathbb{R}^{d,d}$, with $d = 2$ or $d = 3$, is the diffusion–dispersion tensor of the l -th chemical species. If reactive transport in porous media is considered, the water flux $\mathbf{Q}$ and the volumetric water content Θ are typically computed by solving Richards' equation, equipped with appropriate initial and boundary conditions, which (in its mixed pressure formulation) reads as

$$\partial_t(\Theta(\psi)) + \nabla \cdot \mathbf{Q} = 0, \quad \mathbf{Q} = -K(\Theta(\psi)) \nabla(\psi + z). \quad (1.5)$$

In (1.5), ψ is the hydraulic pressure head, $\Theta(\cdot)$ is the given parametrization of the water content, $K(\cdot)$ is the given hydraulic conductivity and z denotes the height against the gravity direction. The applicability and value of the mixed finite element method (MFEM) and its hybrid variant (MHFEM) for solving the systems (1.1)–(1.5), respectively, have been demonstrated in a wide class of works; cf. [2–10] and the references therein. Appreciable advantages of mixed finite element methods are their local mass conservation property (cf. [11,12]) and the fact that they provide an explicit flux approximation as part of the formulation itself which is of particular importance for coupled flow and transport processes as, for instance, given by the set of Eqs. (1.1)–(1.5), where the Darcy flow field $\mathbf{Q}$ of the transport problems (1.1) is calculated from Richards' equation (1.5). While the discretization in space involves a significant set of complexities and challenges, temporal approximations for (highly) transient processes in porous media have received relatively little interest (cf., e.g., [3,7,8,13]) and have been limited to traditional non-adaptive first and second order methods. Rigorous studies of higher order time discretizations are still missing in this field of application even though multiscale phenomena in the time evolution and strongly time dependent processes are often present, for instance, if complex chemical reaction mechanisms arise in Eq. (1.1), such that from the point of view of accuracy of numerical predictions the application of higher order time discretization schemes is recommendable and useful.

The Galerkin method is a known approach to solve time dependent problems; cf. e.g., [14–18]. So far, this variational approach has rarely been used in practice despite of its significant advantages like a uniform variational approach for stability and error analyses, the natural construction of higher order methods, the applicability of goal-oriented error control [19] based on the dual weighted residual approach and the applicability of adaptive finite element techniques for changing the polynomial degree as well as the length of the time intervals. One reason for this might be the higher algorithmic complexity of solving the resulting algebraic systems of equations. Recently, higher order Galerkin time stepping schemes of variational type have been developed and studied for the heat equation [17,20], the nonstationary Stokes and Navier–Stokes equations [15,21,22] and wave problems [16,23,24]. In simulations for benchmarking configurations the efficiency and accuracy of continuous Galerkin–Petrov and discontinuous Galerkin time discretizations were demonstrated [15,16,20–22, 24–26].

Here, we introduce two families of continuous and discontinuous variational time discretization schemes that are combined with mixed finite element approximations of the spatial variables. The class of continuous approximations of the time variable is characterized by a Galerkin–Petrov type approach with piecewise polynomials of order r and, therefore, is referred to as the cGP(r) method. These schemes belong to the classes of A-stable methods [17]. This approach has already been studied in [14] where error estimates have been proved and superconvergence results have been observed. Further error estimates have been provided in [17,26]. The discontinuous variational approximation of the time variable results in a discontinuous Galerkin method with piecewise polynomials of order r . We refer to this approach as the dG(r) method. The resulting numerical schemes are known to belong to the class of strongly A-stable methods [26,27]. Error estimates for the semi-discretization in time of evolution equations of parabolic type are provided in [18]. For the mixed approximation in space we use the Raviart–Thomas family of inf–sup stable pairs of finite elements on quadrilateral and hexahedral elements. The fully discrete approximation schemes are developed by means of a Rothe type approach by discretizing the partial differential equation first in time and then in space. The schemes are studied numerically for a prototype diffusion model only. Their application to more general transport problems, for instance to convection–diffusion–reaction models and systems of equations, is from the algorithmic point of view straightforward. In a forthcoming work [28], an error analysis is presented for the classes of discretization schemes that are considered here. This numerical analysis is currently limited to problems with self-adjoint differential operators. An extension to more general problems is still an ongoing work.

In this work, the solution process of the arising linear systems of equations is described carefully, since this step has shown to be an essential issue in the application of our variational time discretization schemes. This is done for the cGP(2) and dG(1) methods, that are used in this work for the numerical convergence studies and further numerical experiments. The extension of the solution strategy and the construction of efficient preconditioners for still higher order temporal approximations is still an ongoing work. In contrast to former works [3,4,29,30], the mixed finite element approach is applied here in a non-hybrid framework and the linear systems of equations are solved by Schur complement techniques along with nested preconditioned conjugate gradient iterations. This is done due to the experience made by one of the authors with applying hybrid mixed finite element methods to nonlinear problems and coupled systems of equations and the resulting high algorithmic complexity. In this work, to solve the linear systems of equations, the degrees of freedom of the vector-valued variable are eliminated first. In the resulting reduced system of the equations for the cGP(2) and dG(1) approaches,

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