Numerical Analysis of Transport Processes by Means of Discontinuous Galerkin Methods in Space and Time

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Abstract

The presentation is concerned with the numerical treatment of transient transport problems like heat transfer or mass/species transport by means of discontinuous spatial discretization and different time integration schemes. To achieve a semidiscrete initial value problem discontinuous \( p \)-finite elements [1] for the approximation in space are used, where the continuity at the interelement boundaries is just weakly enforced. Furthermore, continuous and discontinuous Galerkin time integration schemes, which evaluate the balance equation in a weak sense over the time interval, are presented [6]. These discretization techniques are investigated with respect to robustness, reliability and accuracy, also in the context of non-smooth initial or boundary conditions. Selected benchmark analyses of heat conduction with an available analytical solution are analyzed for the above described numerical methods. Moreover the highly non-linear reaction-diffusion process of calcium leaching in cementitious materials, which has a major influence on the durability of concrete structures, is modelled by means of the Theory of Porous Media and simulated by spatial and temporal finite element methods.

Keywords: computational mechanics, discontinuous finite element method, Galerkin time integration schemes, heat transfer, calcium leaching

1. Introduction

Transport processes require the transfer of energy and mass from one place to another to satisfy the equilibrium condition. A lot of processes in engineering sciences as well as in natural sciences and a lot of other disciplines are modeled by transport phenomena. Well-known in the classical engineering community are e.g. heat conduction or diffusion processes.

Forward-looking research in the area of thermo-mechanics is currently carried out by a group of engineers who want to obtain a flexibility of the reachable product geometries for metal and plastic materials by a differential thermal process management, cf. [7]. One important part of this project is the numerical treatment of the three manufacture phases, the inductive heating of a blank, the thermo-mechanical forming of the component in the tool and finally the selective air-cooling. All described processes base on the conduction of heat as one special transport phenomenon.

Another ongoing research topic is the durability of concrete structures, which is limited by damage caused by external loading and its interaction with environmentally induced deterioration mechanisms (see e.g. [3]). Model-based prognoses of the degradation of such structures are, in general, founded upon coupled damage models, accounting for the transport of moisture, heat and aggressive substances and the various interactions with diffuse or localized damage. Recent progress in this emerging field of durability mechanics is documented e.g. in [2, 5]. Frequently, diffusion controlled degradation processes are characterized by a pronounced reaction front moving through the structure.

2. Initial boundary value problem of transport phenomena

As a particular example of transport processes the heat conduction due to temperature differences is considered. The local form of the energy balance in terms of the temperature \( \theta(t, X) \) and the tensor valued conductivity coefficient \( \Lambda \) is completed with boundary conditions and initial values to an initial boundary value problem.

\[
\rho c_p \frac{\partial \theta}{\partial t} - \text{div} (\Lambda \cdot \nabla \theta) = Q \quad \forall X \in \Omega, \; \forall t \in [t_0, T]
\]  

(1)

Diffusion phenomena in porous media can also be described by this balance equation, whereby \( \theta \) represents the concentration, \( \Lambda \) the diffusion coefficient and the specific heat capacity \( \rho c_p \) has to be replaced by the porosity \( \phi \).

3. Discontinuous discretization in space

The differential equation form (1) is recast into a weak format by multiplication with a test function and integration over the element domain. In the case of a discontinuous discretization the solutions space as well as the test function are approximated discontinuously with piecewise polynomials. To guarantee the consistency at the interelement boundaries appropriate numerical fluxes have to be generated. The choice
of the flux influences the stability and the accuracy of the algorithm. The numerical fluxes \( \mathbf{A} \cdot \mathbf{\nabla} \theta \cdot \mathbf{n} \) appear in additional terms integrated over the element boundaries compared to the classical finite element analysis in the discontinuous weak form,

\[
\sum_{j=1}^{N} \int_{\Omega} \delta \theta \left[ \dot{\theta} + Q \right] dV + \sum_{i=1}^{N} \int_{\Gamma_D} \delta \theta \left[ \mathbf{A} \cdot \mathbf{\nabla} \theta \right] dA + \sum_{i=1}^{N} \int_{\Gamma_N} \alpha \left\{ \mathbf{A} \cdot \mathbf{\nabla} \theta \cdot \mathbf{n} \right\} dA + \sum_{i=1}^{N} \int_{\Gamma_D} \delta \theta \mathbf{q}^* dA = 0
\]

(2)

where the brackets \( \langle \cdot \rangle \) and \( \langle \cdot \rangle_\perp \) are defined as average and jump, respectively. The finite element approximations and the assembly leads to the linear semidiscrete balance equation of the system.

\[
\mathbf{K} \mathbf{\theta} + \mathbf{D} \mathbf{\dot{\theta}} + [J_{int} + J_D] \mathbf{\theta} = \mathbf{r}_D + \mathbf{r}_N
\]

(3)

4. Galerkin time integration schemes

The foundation of Galerkin time integration schemes lies in the temporal weak formulation of the semidiscrete ordinary differential equation (3) and the temporal finite element approximations of the state variables and the weight functions.

\[
\delta W = \int_{t_n}^{t_{n+1}} \mathbf{w} \cdot \left[ \mathbf{D} \mathbf{\dot{\theta}} + \mathbf{K} \mathbf{\theta} + \mathbf{J} \mathbf{\theta} - \mathbf{r} \right] dt + \mathbf{w}^\top \mathbf{A}_h \left[ \mathbf{\theta}_{n+1}(\mathbf{\theta}^i) \right] = 0
\]

(4)

The weak or strong fulfillment of the continuity of the primary variable \( [\mathbf{\theta}_n] = \mathbf{\theta}^i - \mathbf{\theta}^{i+1} = 0 \) at the border of two time steps \( t_n \) distinguishes between the Galerkin methods in their discontinuous and continuous versions, respectively. Since the discontinuous version of Galerkin integration schemes includes the continuous Galerkin method as a special case, the development of both methods will be described by means of the discontinuous Bubnov–Galerkin method of arbitrary polynomial degree \( p \). For the temporal approximation of the state variables and the weight function LAGRANGE shape functions of arbitrary polynomial degree \( p \) in terms of the natural time coordinate \( \xi_i \in [-1,1] \) are used. The resulting system of equation for discontinuous Galerkin methods with \( i \in [2, p_i+1], j \in [2, p_j+1] \) has to be solved for the temperature increment \( \Delta \mathbf{\theta} \).

\[
\begin{bmatrix}
\mathbf{D}_{ii}^{11} + K_{ii}^{11} + \mathbf{A}_\theta & \mathbf{D}_{ij}^{12} + K_{ij}^{12} \\
\mathbf{D}_{ij}^{12} + K_{ij}^{12} & \mathbf{D}_{jj}^{11} + K_{jj}^{11}
\end{bmatrix}
\begin{bmatrix}
\mathbf{\theta}^i \\
\mathbf{\theta}^j
\end{bmatrix}
= 
\begin{bmatrix}
\mathbf{r}_i^1 + A_\theta \mathbf{\theta}^0 \\
\mathbf{r}_j^1 + A_\theta \mathbf{\theta}^0
\end{bmatrix}
\]

(5)

Herein the time integrals of conduction, capacitance and external heat flux are defined as demonstrated by the following example.

\[
\mathbf{D}_{ii}^{11}(\mathbf{\theta}_{11}) = \left[ N_i^\top(\xi_i) \mathbf{N}_i^\top(\xi_i) \mathbf{D} | J_i | d\xi_i \right]_{-1}^{1}
\]

(6)

Subsequently, the generalized method can be specialized to the continuous Petrov-Galerkin method by enforcing the continuity condition in (5) strongly.

5. Numerical studies

Particular benchmark analyses of linear heat conduction demonstrate the properties of the discontinuous methods with respect to non-smooth initial or boundary conditions. Furthermore, the robustness of the time integration schemes is illustrated due to the pronounced changes of the reaction term and non-smooth changes of Dirichlet boundary conditions of calcium dissolution in cementitious materials. The discontinuous Galerkin method in space and the Galerkin time integration schemes are enriched by error estimates of the \( h \)- and \( p \)-method in order to obtain information on the accuracy of the investigated methods within the context of the presented transport phenomena. Additional detailed information about the introduced topics can be found in [4].

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References


