Higher order variational space-time approximation of wave propagation

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The accurate and reliable numerical approximation of wave propagation is of fundamental importance to the simulation of acoustic, electromagnetic and elastic phenomena. In mechanical engineering, advanced composites such as carbon fibre reinforced polymer have become one of the most promising materials to build light-weight structures for several fields of application, for instance in aerospace and automotive fields, in wind energy, as well as in sailboats, and in modern bicycles, motorcycles and sport cars. These composites are able to combine the high strength and rigidity of the reinforced fiber with excellent properties of synthetic resins in best possible way. Material inspection by piezoelectric induced ultrasonic waves is a relatively new and an intelligent technique to monitor the health of carbon fibre reinforced polymer, for damage detection (delamination, matrix cracks, fibre breaks) and non-destructive evaluation. For the design of structural health monitoring systems it is strictly necessary to understand phenomenologically and quantitatively wave propagation in carbon fibre reinforced polymer and the influence of the geometrical and mechanical properties of the system structure. Numerical simulation is a promising way to achieve this goal. Therefore, the ability to solve numerically the wave equation in three space dimensions is particularly important from the point of view of physical realism. However, this is still a challenging task and an active area of research.

Figure 1: Carbon fibre reinforced polymer.

Recently, Galerkin-type discretization schemes for the temporal variable were proposed and studied for the parabolic heat equation [6] and the Stokes system [3]. The schemes offer significant advantages over finite difference methods for the temporal discretization like a uniform approach for numerical analyses, the natural construction of higher order methods, the applicability of goal-oriented a posteriori error control and of well-known adaptive finite element
techniques. Nevertheless, the higher order variants of these discretization methods lead to complex algebraic systems with block matrix structure that are difficult to solve and required highly adapted iterative solvers. In this contribution continuous and discontinuous variational time discretization schemes for hyperbolic wave equations are presented. This is done for the scalar-valued acoustic wave equation as well as for the vector-valued elastic wave problem. For the discretization in space a symmetric interior penalty discontinuous Galerkin method (SIP-DGM) is used; cf. [4, 5]. In the field of numerical wave propagation the spatial discretization by the discontinuous Galerkin finite element method (DGM) has attracted the interest of researchers; cf., e.g. [2]. Advantages of the DGM are the flexibility with which it can accommodate discontinuities in the model, material parameter and boundary conditions and the ability to approximate the wavefield with high degree polynomials. The DGM has the further advantage that it can accommodate discontinuities also in the wavefield, it can be energy conservative, and it is suitable for parallel implementation. The mass matrix of the DGM is block-diagonal, with block size equal to the number of degrees of freedom per element, such that its inverse is available at low computational cost.

As a prototype equation we consider elastic wave propagation described by

\[
\begin{align*}
\rho \frac{\partial^2 u}{\partial t^2} - \nabla \cdot \sigma(u) &= f, \\
\mathbf{u}(0) &= \mathbf{u}_0, \quad \partial_t \mathbf{u}(0) = \mathbf{v}_0, \\
\mathbf{u}(t) &= \mathbf{u}_D \text{ auf } \partial \Omega_D, \quad \sigma(u)n = t_N \text{ auf } \partial \Omega_N
\end{align*}
\]

supplemented by Hook’s law of linear elasticity

\[
\begin{align*}
\sigma(u) &= C\varepsilon(u), \quad \varepsilon(u) = \left(\nabla u + (\nabla u)^\top\right)/2, \quad \sigma_{ij} = C_{ij}(x) : \nabla u.
\end{align*}
\]

Two families of continuous and discontinuous variational time discretization schemes are introduced and studied. For this, the following time-discrete function spaces are needed:

\[
\begin{align*}
\mathcal{X}^r(J; X) &:= \left\{ u \in C(I; X) \mid u_{|I_n} \in P_r(I_n; X), \ \forall n \right\} \\
&\subset \left\{ u \in L^2(I; X) \mid d_t u \in L^2(I; X^*) \right\} \\
\mathcal{Y}^r(J; X) &:= \left\{ u \in L^2(I; X) \mid u_{|I_n} \in P_r(I_n; X), \ \forall n \right\} \\
P_r(J; X) &:= \left\{ u : J \rightarrow X \mid u(t) = \sum_{j=0}^{r} \xi_n^j \nu^j, \ \xi_n^j \in X, \ \forall j \right\}
\end{align*}
\]

We introduce the auxiliary variable \( \mathbf{v} = \partial_t \mathbf{u} \). Then, in the case of a continuous time approximation we are led to the semidiscrte approximation scheme:
Find \( u_\tau \in \mathcal{X}(V) \) and \( v_\tau \in \mathcal{X}(V) \) such that \( u_\tau(0) = u_0 \), \( v_\tau(0) = v_0 \) and

\[
\int_0^T \left\{ \langle \rho \partial_t u_\tau(t), \tilde{w}_\tau(t) \rangle - \langle \rho v_\tau(t), \tilde{w}_\tau(t) \rangle \right\} dt = 0
\]

\[
\int_0^T \left\{ \langle \rho \partial_t v_\tau(t), \tilde{w}_\tau(t) \rangle + \langle a(u_\tau(t), \tilde{w}_\tau(t)) \rangle \right\} dt = \int_0^T \langle f(t), \tilde{w}_\tau(t) \rangle dt
\]

for all \( \tilde{w}_\tau \in \mathcal{Y}^{-1}(V) \), \( \tilde{w}_\tau \in \mathcal{Y}^{-1}(V) \).

In terms of the representation by means of finite element basis functions (cf. [4])

\[
\begin{align*}
   u_\tau(t) &= \sum_{j=0}^r U_n^j \xi_n,i(t), \\
   v_\tau(t) &= \sum_{j=0}^r V_n^j \xi_n,i(t)
\end{align*}
\]

and with the basis of test functions

\[
\begin{align*}
   w_\tau(t) &= \begin{cases} 
      w \zeta_n,i(t), & \text{on } I_n = [t_{n-1}, t_n] \\
      0, & \text{on } I \setminus I_n
   \end{cases}
\end{align*}
\]

we get the following semidiscrete approximation scheme:

Find pairs \( \{u_\tau|_{I_n}, v_\tau|_{I_n}\} \in \mathbb{P}_r(I_n; V) \times \mathbb{P}_r(I_n; V) \), with coefficients \( U_n^j, V_n^j \in V \), \( j = 1, \ldots, r \), such that

\[
\begin{align*}
   \sum_{j=0}^r \left\{ \alpha_{i,j} \langle \rho U_n^j, \tilde{w} \rangle - \beta_{i,j} \langle \rho V_n^j, \tilde{w} \rangle \right\} &= 0 \\
   \sum_{j=0}^r \left\{ \alpha_{i,j} \langle \rho V_n^j, \tilde{w} \rangle + \beta_{i,j} a(U_n^j, \tilde{w}) \right\} &= \sum_{i=0}^r \beta_{i,j} \langle F_n^i, \tilde{w} \rangle
\end{align*}
\]

for all \( \tilde{w}, \tilde{w} \in V \) and \( i = 1, \ldots, r \), and all intervals \( I_n = (t_{n-1}, t_n] \), \( n = 1, \ldots, N \) with \( U_n^0 = U_{n-1}^r, V_n^0 = V_{n-1}^r \).

The coefficients are defined by:

\[
\begin{align*}
   \alpha_{i,j} &= \langle \xi_n,i, \zeta_n,i \rangle_{L^2(I_n)} = \int_I \xi_j^\prime(t) \zeta_i(t) \, dt \\
   \beta_{i,j} &= \langle \xi_n,i, \zeta_n,i \rangle_{L^2(I_n)} = \int_I \xi_j(t) \zeta_i(t) \tau_n \, dt
\end{align*}
\]

The discretization in space by the SIP-DGM method now follows the usual way of applying finite element methods. For the technical details we refer to [4, 5]. For \( r = 2 \), corresponding to an approximation of the time variable with piecewise quadratic polynomials, we end up with the following linear system of equations for each subinterval \( I_n \), with \( n = 1, \ldots, N \):

3
By elimination of internal degrees of freedom and computing the Schur complement we are led to the following solution algorithm:

$$S \mathbf{u}_n^2 = \beta \mathbf{b}_n^1 + \left( \mu_1 M + \frac{\tau^2}{4} A \right) M^{-1} \mathbf{b}_n^0$$

$$S = \alpha \beta M + \left( \mu_1 M + \frac{\tau^2}{4} A \right) M^{-1} \left( \mu_2 M + \frac{\tau^2}{4} A \right)$$

$$\mathbf{u}_n^1 = \frac{1}{\beta} M^{-1} \left( \left( \mu_2 M + \frac{\tau^2}{4} A \right) \mathbf{u}_n^2 - \mathbf{b}_n^2 \right)$$

The linear system for the unknown coefficient vector $\mathbf{u}_n^2$ is solved by nested CG iterations (cf. [5]). The implementation of this variational space-time approach to wave problems was done in the opensource software library deal.ii (cf. [1]).

Basic features of our software platform are summarized in the following:

- Parallel Finite Element Toolbox: deal.II 8.1.0
- Parallel Grid Partitioner, Graph handling: p4est 0.3.4.2
- Parallel Linear Algebra: Trilinos 11.8.x
- Parallel File-IO: HDF5/XDMF (or PVTU)
- MPI: MPICH/MVAPICH (infiniband), OpenMPI
- C++/C++1x: gcc 4.9.0, clang 3.4
\[
C(x) := \begin{cases} 
C_0 = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}, & x \in \Omega \setminus \Omega_1 \\
\bar{C}_1 := \begin{pmatrix} 7.5 & 2.5 \\ 2.5 & 7.5 \end{pmatrix} \equiv \begin{pmatrix} 5 & 0 \\ 0 & 10 \end{pmatrix}, & x \in \Omega_1 
\end{cases}
\]

with \( \Omega_1 := \{ x \in \mathbb{R}^2 \mid -x_1 \leq x_2 \leq -x_1 + 2 \} \) and \( f(x, t) = \sin(\omega t) p(x) \) in \( \Omega_A \).

![Figure 2: Test setting and calculated profile for wave propagation in an anisotropic and heterogeneous medium.](image)

- Automated Build System: candi for DTM++.TOOLBOX
  git clone https://github.com/koecher/candi
- Frontend Simulation Software: DTM++

The accuracy and performance properties of the methods are illustrated by numerous convergence studies and complex three-dimensional problems that are of practical interest in the field of structural health monitoring. For acoustic wave problems the impact of material anisotropy and heterogeneity is further studied carefully.

Finally, the application of goal-oriented a-posteriori error control by a dual weighted residual approach along with space-time mesh adaptivity is illustrated. This is done for a class of convection-dominated transport problems with sharp interior and boundary layers (cf. [7, 8]). Our current experiences in applying these techniques are expected to be fruitful for the future implementation of goal-oriented a-posteriori error control mechanisms for higher order approximations of wave propagation phenomena which will be next stage of completion of our software platform.

References

Figure 3: Goal-oriented error control for stabilized approximations of convection-dominated problems (cf. [7]).


