On the Numerical Solution of Advection-Diffusion-Reaction Equations: Time-Discontinuous Galerkin and Finite Calculus Methods

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Keywords: advection-diffusion-problems, bone fracture healing, time-discontinuous Galerkin methods, Finite Increment Calculus method.

SUMMARY. An algorithm is introduced, which provides stabilised solutions for a system of multiple coupled transient non-linear advection-diffusion-reaction equations. The time integration for several time scales is handled by a time-discontinuous Galerkin scheme (TDG), while the necessary stabilisation is provided by the Finite Increment Calculus method (FIC-FEM).

The advection-diffusion-reaction equation describes the movement and conversion e.g. of chemical or biological entities and the evolution of their concentration distribution. The generalized transient advection-diffusion-reaction equation in one dimension reads

\[
\frac{\partial u}{\partial t} = -a(x, t) \nabla u + \nabla (d(x, t) \nabla u) + r(x, t)u, \tag{1}
\]

which has to be solved for \( u(x, t) \) in a domain \( \Omega \) with the initial condition \( u(x, 0) = u_0 \) in \( \Omega \) and boundary condition \( u = g \) at \( \Gamma = \partial \Omega \). The parameters \( a(x, t) \), \( d(x, t) \) and \( r(x, t) \) describe the advection, diffusion and reaction coefficients, respectively.

It is well known, that the solution of equation (1) using a standard Galerkin approach is often polluted by spurious oscillations, which appear in the vicinity of steep gradients of the solution and/or are caused by dominant advection or reaction terms. This behaviour initiated a long lasting discussion on the numerical treatment of these problems. Within today’s literature there are numerous suggestions how to treat the specific difficulties (e.g. Streamline Upwind Petrov Galerkin Method, Subgrid Scale Methods, Flux-Corrected Transport). Additionally a broad variety of numerical schemes for the temporal discretization of the advection-diffusion-reaction equation have been discussed so far; based on finite difference methods, finite volume methods or finite element methods and classified into implicit schemes (Backward Euler, Crank-Nicholson) and explicit schemes (Euler Forward, Lax, Leapfrog, etc.). It is well known that the solution strongly depends on the Courant- and Peclet-Numbers, which describe the problem dependent ratio between temporal and spatial discretization and the advection-diffusion ratio.

However, serious problems remain when solving systems of coupled advection-diffusion-reaction problems where different advection coefficients and different ratios between advection and diffusion coefficients are present. The complexity becomes even greater, when these coefficients are not constant but change in space and time.

It will be shown, that Time Discontinuous Galerkin (TDG) method is insensitive with regard to the Courant criterion. This enables the treatment of coupled problems by usage of the same temporal and spatial discretization without loss of accuracy. Due to this insensitivity different timescales
within the coupled system can be solved comfortably and no further effort has to be made, i.e. adaption of timesteps or meshsize.

Furthermore, the Finite Increment Calculus Method (FIC-FEM) [1] is applied, in order to stabilise the computation and suppress spurious oscillations, thus preventing the appearance of unphysical values within the solution (e.g. negative concentrations). The FIC-FEM offers a physically meaningful access to stabilisation techniques and is applicable for the complete range of parameter values, i.e. even when some coefficients are zero.

The application of the proposed computational approach will be demonstrated exemplarily on a model for fracture healing [2] based on cell migration and proliferation, which is described by a set of several coupled advection-diffusion-reaction equations. By these equations the complicated biochemical evolution and communications processes are presented, i.e. bone marrow cells differentiate in dependence of the biochemical environment to bone cells, fibrous tissue cells or cartilage cells. Biochemical signals are send out for support of endothelial cells for example to ensure nutrient transport via vascularization. The random movement of cells and molecules is described by the diffusion term, the chemo- and haptotactic attraction takes the form of an advective part and finally the propagation, dying and differentiation of cells, extracellular matrix and messenger molecules is depicted by reactive terms. As an example figure 1 shows the evolution of bone matrix distribution inside the callus within the first ten days after the fracture occured. The callus is very roughly represented.

The advantages of the suggested TDG-FIC-Method will be demonstrated and applied to the briefly outlined fracture healing model.

Acknowledgements: This research project is funded by the German Research Foundation (DFG-NA 330/8-1). The authors gratefully acknowledge the financial support.

References
