

Application of fully implicit Nested Newton solvers to multicomponent multiphase flow in porous media and to elastoplastic deformations of biological tissue

Markus M. Knodel¹

Advanced models of complicated physical and biological processes incorporate huge equation systems which combine partial differential equations (PDEs), ordinary differential equations (ODEs), and algebraic equations (AEs).

The monolithic solution of such extended equation systems all together using standard techniques sometimes is very time consuming due to the highly nonlinear couplings linking the PDEs, ODEs, and AEs. The application of operator splitting methods as well often is highly time consuming, as very small time steps often are needed in such cases.

The application of nested Newton solvers allows to shift a substantial part of the nonlinear computations to the so-called local system containing only non-spatially coupling equations (ODEs, AEs). The global equations contain all PDEs and are hence spatially connected. If the local variables are coupled with the global variables by means of a so-called resolution function, the solution technique remains monolithic and fully implicit. The number of the local Newton steps (which can be performed with perfectly parallel scalability) displays an upper bound for the global Newton steps, which contain the spatial couplings.

We present two examples of applications of a nested Newton algorithms which allow the efficient evaluation of the corresponding models:

In order to study the efficiency of the various forms of trapping including mineral trapping scenarios for CO₂ storage behaviour in deep layers of porous media, we apply the globally fully implicit PDE reduction method developed 2007 by Kräutle and Knabner for one-phase flow extending the method to the case of an arbitrary number of gases in gaseous phase. The advective parts of the Finite Element discretized PDEs are stabilized with cell centered Finite Volumes. We present scenarios of the injection of a mixture of various gases into deep layers, we investigate phase change effects in the context of various gases, and study the mineral trapping effects of the storage technique.

Further, we simulate elastoplastic deformation of biological tissue with anisotropic structure in case of a highly nonlinear material model developed by Di Stefano and Grillo. Applying the BilbyKrönerLee (BKL) multiplicative decomposition of the deformation gradient into an elastic and a plastic part, a natural split into local and global system is achieved. The PDEs representing the virtual powers are discretized by means of Finite Elements. We compare the simulations for the case of isotropic and anisotropic material and find substantial differences in the properties of the material stress response depending on the velocity of the material deformation.

Our applications demonstrate the potential of nested Newton procedures for efficient solution techniques in case of highly nonlinear models of complicated scenarios.

References:

[1] Knodel, Kräutle, Knabner. *Comput Geosci* 2022. doi.org/10.1007/s10596-022-10140-y

¹Goethe-Universität Frankfurt am Main, Goethe Center for Scientific Computing
markus.knodel@gcsc.uni-frankfurt.de