AN ADAPTIVE, PROCESS-PRESERVING MODIFIED NEWTON'S METHOD TO SOLVE REACTIVE MULTICOMPONENT TRANSPORT PROBLEMS EFFICIENTLY

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ABSTRACT

The development of versatile hydrogeochemical mulitcomponent transport simulation tools that handle the variety of coupled hydraulic, chemical, and biological processes, which are relevant for the fate of contaminant plumes in porous media, accurately and efficiently, is still a demanding task. The general coupled PDE/ODE system for reactive multicomponent transport in the solid and aqueous phase reads

$$\partial_t(\Theta c_i) - \nabla \cdot (\boldsymbol{D}\nabla c_i - \boldsymbol{q}c_i) = \Theta \sum_{r=1}^{N_R} \nu_{ir} R_r , \quad \text{and} \quad \partial_t(c_j) = \sum_{r=1}^{N_R} \nu_{jr} R_r ,$$

with time $t \in (0, T)$, $x \in \Omega \subset R^d$, $d \in \{1, 2, 3\}$, volumetric water content $\Theta(x, t)$, the solute concentration $c_i(x, t)$. $c_j(x, t)$ is the concentration of immobile species, $\boldsymbol{D}(x, t)$ the diffusion–dispersion–tensor, and $\boldsymbol{q}(x, t)$ the specific discharge. The equations are coupled with each other via the reaction rates R_r that account, e.g., for natural degradation processes of organic contaminants or kinetic reactions according the law of mass action. A popular approach to solve this problem class is to decouple reaction and transport parts. This allows to reduce the computational burden, to apply specific solution techniques for the subproblems and even to use existing codes for them, but introduces a consistency error which however can vanish, e.g., for models with linear reaction terms independent of space, and a divergence free flow field [1]; situations, though, that are of limited practical relevance.

Thus we investigate further the global implicit solution approach for the above system that treats subprocesses simultaneously, apply Newton's method with Armijo's rule as nonlinear solver and develop new efficient solution strategies by modifying the Jacobian of the problem. This leads to decoupled blocks in the Jacobian that can be solved independently from each other. As even in large chemical systems typically only few species are directly coupled in one reaction, the resulting sparse matrix structure in the finite element matrix can be exploited to reduce the computational effort. After the variational formulation of the coupled nonlinear systems of parabolic partial and ordinary differential equations

a H^1-conforming finite element discretization in space with linear ansatz functions is pursued, combined with the implicit Euler method or the BDF-2 scheme in time. A nonlinear equation system of the dimension $(N + 1) \times N_S$ results (N: DOF in space, N_S: number of species). When numbering the DOF nodewise (in the order of the elements), in the Jacobian at each node block matrices of dimension $N_S \times N_S$ occur, containing the partial derivatives of the discretized problem according to the species concentrations. Those are essentially the derivatives of the reaction terms, which read, e.g., for geochemical kinetic reaction rates according to the mass action law:

$$\frac{\partial R_r}{\partial c_k} = k_r^b (-\nu_{kr}) c_k^{(-\nu_{kr}-1)} \prod_{i \neq k} c_i^{-\nu_{ir}}$$

(with stoichiometric factor $\nu_{kr} < 0$, product concentration c_k, and k_r^b as the backward reaction rate constant), for other rates as degradation according to multiple Monod kinetics see [1]. As not all of the species are coupled by reactions to each other, through an analysis of the reaction network reducible matrix parts can be identified – even in course of the simulation – and solved seperately. This is the key point to reduce the computational effort while at the same time solving the global implicit problem in one Newton step.

The reducability of the Jacobian can also be enforced by the neglection of weak coupling terms which arise when small reaction rate constants or small concentrations occur. This corresponds to a modified Newton's method, then. As the correct right-hand-side of the problem is assembled, the solution still converges to the correct, process-preserving (coupled) solution. If the convergence properties of the Newton scheme are not deteriorated substantially, a clear gain in efficiency can be reported. The Damköhler number can be a criterium for the decision to neglect reaction terms.

An academic 16 species example in 1D, where the band structure is very favorable, reveals the potential of the method, with a speed up of factor ≈ 93 in the direct linear solver and 9 in total CPU time. Another 12 species examples according to [1,3] showed speed ups of factor 37 in the linear solver and 4 in total. A real world EDTA degradation example [2] which has been used in the literature to test implementations of reactive multispecies models has been solved with this technique also.

In 2D the matrix structure is less optimal as the band width is broader and a direct solver probably is not competitive. Thus the potential efficiency gain is only of order N_p instead of N_p^2 (where N_p is the number of equal parts the Jacobian is split in). For iterative solvers however the iteration number may differ for the matrix parts, what can be an additional gain. The method has been implemented with a fully adaptive algorithm analysing the connectivity graph of the Jacobian in potentially each time step. Experiments with the above 12 species example using BiCGStab as linear solver also showed promising results with accelerations of factor 4 in the solver part.

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