Report No.
UCB/SEMM-2003/06

Structural Engineering,
Mechanics and Materials

1-D Diffusion Deformation Phenomena: Accuracy Analysis of Operator Splitting

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October 2003

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October 7, 2003

SUMMARY

This report provides the details of analysis of orders of accuracy of operator splitting time stepping schemes, applied to coupled problems. The phenomenon considered is solvent diffusion in a deforming polymer, where diffusion and deformation are coupled. Operator splitting is applied to a set of Differential Algebraic Equations (DAEs) arising from spatial discretization of the equations governing the coupled phenomenon. Although, solvent concentration and polymer deformation are natural choices of the fields held fixed, respectively, in the two phases of the split, complications arise when a formulation in terms of solvent activity instead of concentration is chosen. In this paper, analysis of order of accuracy of "adiabatic splitting", a particular operator splitting scheme, with activity and polymer deformation as the primary variables, is presented. It is shown that adiabatic splitting is globally first order accurate on DAEs in the present case, where activity and polymer deformation are the primary variables.

KEYWORDS: Operator Splitting; Fractional step methods; Differential-Algebraic-Equations; Error Order; Nonlinear Coupled Problem, Diffusion-deformation Coupling.

1 Introduction

Adiabatic splitting, a particular operator splitting technique, is applied in the context of thermo-elasto-plasticity (see e.g., Armero and Simo [1992],

Armero and Simo [1993]). In these references, accuracy analysis of the dynamic case, which leads to a set of ordinary differential equations (on spatial discretization) is presented. However, our coupled governing equations for the diffusion-deformation phenomenon, although similar to the thermo-elasto-plasticity case, are different in that they correspond to the quasi-static case. Spatial discretization of the coupled equations for the quasistatic case leads to DAEs instead of ODEs. Results of order analysis of operator splits for generic DAEs are presented in Vijalapura and Govindjee [2003a]. These results can be utilized directly when solvent concentration and polymer deformation are used as primary variables, with the polymer deforming elastically. However, details of the order analysis when the governing equations are formulated in terms of solvent activity and polymer deformation is not obvious. This report provides the details of such an analysis. The important case of viscoelastic polymer deformation (the elastic case being the special case) coupled to diffusion is also included. In the following sections, governing equations for the diffusion-deformation phenomenon, their spatial discretization, and order analysis of operator splitting on the resulting DAEs, are presented.

2 Governing Equations

The balance laws and a specific set of constitutive relations defining our diffusion-deformation model in 1-D are summarized in this section. Additional discussion of the model equations can be found in Vijalapura and Govindjee [2003b].

Solvent Mass Balance:

$$\frac{dM}{dt} = -\frac{df(\phi,\, M)}{dX} \quad X \in \Omega = (0,\, L). \tag{1}$$

Here, M is the solvent concentration (solvent mass per unit undeformed polymer length), ϕ denotes the polymer deformation, f is the solvent flux and t and X denote the time and position variables. The polymer occupies a reference configuration Ω.

MIXTURE STRESS EQUILIBRIUM:

$$\frac{d\sigma(\phi,\, M)}{dX} = 0. \tag{2}$$

Here, σ denotes the mixture stress and Eqn. (2) corresponds to the quasi-static case where inertial effects are neglected. The stress depends on ϕ through the stretch $\lambda = \partial\phi/\partial X$. These balance laws are supplemented by appropriate boundary conditions.

$$\sigma\, n = \bar{\sigma} \quad X \in \partial_\sigma\Omega; \quad \phi = \bar{\phi} \quad X \in \partial_\phi\Omega \tag{3}$$

$$M = \bar{M} \text{ (or } A = \bar{A}) \quad X \in \partial_M\Omega; \quad f\, n = \bar{f} \quad X \in \partial_f\Omega. \tag{4}$$

For the deformation problem, the boundary conditions are in terms of specified deformations $\bar{\phi}$ or tractions $\bar{\sigma}$, while for the diffusion problem, fluxes $\bar{f}$ or concentrations $\bar{M}$ can be specified. An additional important mixed boundary condition in terms of activity A which is a function of ϕ and M can also be specified for the diffusion problem.
The constitutive relations for the flux f, mixture stress σ, and the chemical potential μ complete the balance laws for the diffusion-deformation problem. For the mixture stress, we assume,

$$\underbrace{\sigma}_{Total} = \underbrace{\sigma_s(M,\, \lambda)}_{Solvent} + \underbrace{\sigma_p^\infty(\lambda)}_{Elastic} + \underbrace{q}_{Viscous}, \tag{5}$$

where, σ_s is a contribution due to solvent presence which induces swelling, σ_p^∞ is the elastic contribution, and q is the viscoelastic contribution from the polymer skeleton. The purely elastic case corresponds to setting $q = 0$. The functional forms for σ_s, σ_p^∞ are given by,

$$\begin{aligned} \sigma_s &= E_s \ln\left[\frac{bh(\lambda)}{h(\lambda) - M}\right], \\ \sigma_p^\infty &= \frac{1}{2}E^\infty(\lambda - 1)\left[1 + \frac{f_0}{(1 - f_0)h(\lambda)}\right]. \end{aligned} \tag{6}$$

Further, the viscoelastic over stress is assumed to be given by a first order evolution law with a concentration dependent relaxation time τ.

$$\frac{dq}{dt} + \frac{q}{\tau(M,\, \lambda)} = \beta\frac{d}{dt}[\sigma_p^\infty]. \tag{7}$$

In Eqns. (6) and (7), the moduli E_s, E^∞, and the parameters f_0, b are constants. Further, h is a linear function of the stretch λ. In the above relations specifying the stress, the coupling where diffusion affects deformation is introduced through σ_s and τ.
For the diffusion problem, the flux law is specified by,

$$f = -B(m)\frac{M}{\lambda^2}\frac{d\mu}{dX}, \tag{8}$$

where, B is a mobility coefficient depending nonlinearly on the spatial concentration, $m = M/\lambda$, and μ is the chemical potential of the solvent in the mixture. The chemical potential is constitutively specified as:

$$\frac{\mu}{RT} = \ln(bM) - \ln(h(\lambda) - M) := \log A. \tag{9}$$

Here, T denotes absolute temperature which is fixed assuming isothermal conditions, and R is the universal gas constant. Equation (9) for μ also defines activity A. In specifying the flux law, the coupling where deformation affects diffusion is introduced strongly through the chemical potential and mildly through the mobility coefficient. Functional forms of the remaining quantities are summarized in the Table 1.

Table 1: Choice of functions for mobility coefficient,the relaxation time, and the current free volume

	Functional Form	Parameters
Diffusion Coefficient B	$B(m(M,\,\lambda)) = B_0(1 + \xi(M/\lambda)^2)/RT$	B_0, ξ
Relaxation Time τ	$\tau(m(M,\,\lambda)) \;= \tau_0 g(M,\,\lambda)$	τ_0
Relaxation Time Function g	$g(M,\,\lambda) = \exp(B_d(\hat{f} - f_0)/(f_0\hat{f}))$	B_d
Current Free Volume $\hat{f}$	$\hat{f}(M,\,\lambda) \;= f_0 + a_\eta M/\lambda$	a_η

Remark 1
Spatial discretization of the solvent mass balance (1) results in a first order system of ODEs in variables defining the discretized concentration field. On

the other hand, spatial discretization of mixture stress equilibrium (2) results in algebraic constraints between deformation and concentration variables. This immediately leads to the canonical setting given in (Vijalapura and Govindjee [2003a], section 2.2). If one wishes to use activity as the primary variable instead of concentration, additional issues must be addressed. As this is an important practical issue, the details of using activity as a primary variable are considered in section 3. □

3 Activity and Deformation Formulation

3.1 Spatial Discretization

Spatial discretization is performed using standard C^0 finite elements (see e.g., Hughes [2000]) for the spatial fields. The displacement field u defined as $u = \phi(X) - X$ is interpolated linearly in terms of nodal variables $\mathbf{U}$. Similarly, either the concentration M or activity A can be linearly interpolated in terms of their nodal values. When concentration Dirichlet boundary conditions are specified, the field M is interpolated. When activity Dirichlet boundary conditions are specified, the activity field A is interpolated. Activity interpolations are natural for imposing activity conditions. Furthermore, they avoid the need for computing the spatial derivative of stretch λ that appears through the spatial derivative of the chemical potential μ in the mass balance equations. In the following, activity interpolation is considered in terms of nodal activities $\mathbf{A}$ along with activity boundary conditions.
The Galerkin finite element method can be stated as: Find the C^0 fields, u and A (or equivalently, $\mathbf{U}$ and $\mathbf{A}$) satisfying (10)and (11) for all admissible variations δu and δA.
Mass Balance:

$$\begin{aligned} G_A(A,u;\delta A) = &\int_0^1 \frac{dM(A,\,\lambda)}{dt}\,\delta A\,dX \\ &+ \int_0^1 B(M(A,\lambda),\lambda)\frac{1}{A}\frac{dA}{dX}\frac{d(\delta A)}{dX}\,dX - \bar{f}\delta A\,|_{\partial_f\Omega} = 0. \end{aligned} \tag{10}$$

Here, the admissible activity variations satisfy $\delta A = 0$ on $\partial_A\Omega$.
Momentum Balance:

$$G_u(A,u;\delta u) = \int_0^1 \sigma(A,\,\lambda)\,\frac{d(\delta u)}{dX}\,dX - \bar{\sigma}\delta u\,|_{\partial_\sigma\Omega} = 0. \tag{11}$$

The stretch λ is calculated from the interpolation field u which is obtained from the nodal values $\mathbf{U}$. The admissible displacement variations satisfy $\delta u = 0$ on $\partial_u \Omega$.
Since, the weak forms (10) and (11) hold for all admissible variations δA and δu, one can write the following sets of DAEs, indicated in terms of their functional dependencies.

$$\text{Mass Balance:} \quad \frac{d\mathbf{M}(\mathbf{A},\mathbf{U})}{dt} + \mathbf{R}(\mathbf{A},\mathbf{U}) = \mathbf{f}, \tag{12a}$$

$$\text{Momentum Balance:} \quad \mathbf{S}(\mathbf{A},\mathbf{U},\mathbf{q}) - \mathbf{s} = \mathbf{0}. \tag{12b}$$

The various matrices are given by,

$$\mathbf{M}(\mathbf{A},\mathbf{U}) = \mathop{\mathsf{A}}_{e=1}^{n_{el}} \bar{\mathbf{m}}^{(e)}_{[2\times 1]} : \quad \bar{\mathbf{m}}^{(e)}_{(A,1)} = \int_{L_e} N^A M(\mathbf{A},\mathbf{U}) dX, \tag{13}$$

$$\mathbf{R}(\mathbf{A},\mathbf{U}) = \mathop{\mathsf{A}}_{e=1}^{n_{el}} \mathbf{r}^{(e)}_{[2\times 1]} : \quad \mathbf{r}^{(e)}_{(A,1)} = \int_{L_e} \frac{dN^A}{dX} \frac{B(\mathbf{A},\mathbf{U})}{A} \frac{dA}{dX}\, dX, \tag{14}$$

$$\mathbf{S}(\mathbf{A},\mathbf{U},\mathbf{q}) = \mathop{\mathsf{A}}_{e=1}^{n_{el}} \mathbf{s}^{(e)}_{[2\times 1]} : \quad \mathbf{s}^{(e)}_{(A,1)} = \int_{L_e} \frac{dN^A}{dX} \sigma(\mathbf{U},\mathbf{A},\mathbf{q})\, dX. \tag{15}$$

In Eqn. (12b), the explicit dependence of the residual on the viscoelastic overstress q is shown. In an actual implementation, the various integrals are computed using numerical quadrature and viscoelastic stresses need only be computed at the quadrature points. Their evolution at the quadrature points is given by (7) resulting in a system of ODEs, and their values at quadrature points can be stacked into one vector $\mathbf{q}$. Thus, in the viscoelastic case, the evolution of the viscoelastic stresses together with the spatially discrete mass balance equations, form a system of ODEs. These ODEs together with the algebraic constraints due to mixture equilibrium (Eq. (12b)), give rise to DAEs which can be put in the canonical form, presented in Vijalapura and Govindjee [2003a].
In this reference, it is also shown that both one and two pass algorithms are only globally first order accurate. Therefore, only one pass algorithms are considered and the system of ODEs are discretized using Backward Euler which also renders first order global accuracy.

3.2 Implementation of the Monolithic Algorithm

The monolithic scheme for time stepping from t_n to t_{n+1} can be summarized as solving for $\mathbf{q}_{n+1}$, $\mathbf{A}_{n+1}$ and $\mathbf{U}_{n+1}$ given their values at t_n.

Mass Balance:

$$\frac{\mathbf{M}(\mathbf{A}_{n+1}, \mathbf{U}_{n+1}) - \mathbf{M}(\mathbf{A}_n, \mathbf{U}_n)}{\Delta t} = -\mathbf{R}(\mathbf{A}_{n+1}, \mathbf{U}_{n+1}) + \mathbf{f}_{n+1}, \tag{16a}$$

Momentum Balance:

$$\mathbf{S}(\mathbf{A}_{n+1}, \mathbf{U}_{n+1}, \mathbf{q}_{n+1}) - \mathbf{s}_{n+1} = \mathbf{0}, \tag{16b}$$

Viscoelastic Evolution:

$$\frac{q^{(i)}_{n+1} - q^{(i)}_n}{\Delta t} + \frac{q^{(i)}_{n+1}}{\tau(M_{n+1},\, \lambda_{n+1})} = \beta \frac{\sigma_p^{\infty} \mid_{t_{n+1}} - \sigma_p^{\infty} \mid_{t_n}}{\Delta t}. \tag{16c}$$

It is important to observe that the unknown nodal activities and displacements form the driving variables. In Eqn. (16c), the index i runs from 1 to the number of quadrature points. The implementation details are straight forward and the reader may wish to consult Vijalapura and Govindjee [2003b] for further details on the monolithic scheme in the context of a second order Backward Differentiation Formula (BDF2).

3.3 Implementation of the Splitting Algorithm

The splitting algorithm presented here constitutes the so-called adiabatic split (see Armero and Simo [1992] for its implementation in the context of thermomechanical problems). For future reference, this algorithm will be labeled ALGO1. A stability analysis is also provided in this reference. However, analysis of global orders of accuracy is missing for the quasistatic case. The various implementation steps are summarized below. A derivation on the global orders of convergence is provided later. The splitting involves two evolution operators, one for deformation and one for solvent concentration.

Deformation Phase: ($\dot{\mathbf{M}} = \mathbf{0}$)

1. Given $\mathbf{U}_n$ and $\mathbf{A}_n$ at time t_n, calculate the concentration field M_n from (9). Since the stretch λ is only piecewise continuous, so is M_n.

2. Solve for $\mathbf{U}_{n+1}$ from mixture stress equilibrium (16b) by holding M_n fixed pointwise in the interior of each element. In particular, M_n is

held fixed while calculating the contribution from solvent stress σ^s and viscoelastic stress q from the element interiors. Fixing M_n is a special case of fixing $\mathbf{M}_n$ (i.e., $\dot{\mathbf{M}} = \mathbf{0}$), a fact that is used in the analysis later.

3. The visco-elastic stresses are evolved in this phase, with M_n fixed.

Remark 2
Since in the spatially continuous case, activity A depends both on M and λ, keeping M fixed and evolving λ also evolves the activity field. However, in the spatially discrete setting, this evolved, intermediate activity field need not be C^0 nor explicitly calculated. □

Diffusion Phase: $(\dot{\mathbf{U}} = \mathbf{0})$

1. The displacement $\mathbf{U}_{n+1}$ is frozen ($\dot{\mathbf{U}} = \mathbf{0}$). Nodal activity $\mathbf{A}_{n+1}$ is obtained by solving (16a), using $\tilde{M}_{n+1} = M_n$ as the needed initial condition for time stepping. Here, $\tilde{(\cdot)}$, denotes an intermediate quantity after the first of the two fractional steps. It is important to note that the activity at the end of the deformation phase is never needed. Furthermore, the viscoelastic stresses are frozen in this phase; see Remark 9. □

3.4 Order of Accuracy

Because of the unusual details of an adiabatic split, one needs to re-examine the issue of accuracy and convergence. To aid in this analysis, we first start with the derivation of an abstract result, independent of split algorithms.
Lemma 1: Given an index 1 DAE

$$\begin{pmatrix} \mathbf{0} \\ \dot{\mathbf{Y}} \end{pmatrix} = \begin{pmatrix} \mathbf{G}(\mathbf{X}, \mathbf{Y}) \\ \mathbf{F}(\mathbf{X}, \mathbf{Y}) \end{pmatrix} \tag{17}$$

(i.e., $\mathbf{G}(\mathbf{X}, \mathbf{Y}) = 0 \implies \mathbf{X} = \mathbf{H}(\mathbf{Y})$) that satisfies a Lipschitz condition $\|\mathbf{D_Y F}(\mathbf{H}(\mathbf{Y}), \mathbf{Y})\| < L$, the one-step algorithm

$$\frac{\mathbf{Y}_{n+1} - \mathbf{Y}_n}{\Delta t} = \mathbf{F}(\mathbf{H}(\mathbf{Y}_n) + \mathbf{e}_n \Delta t, \mathbf{Y}_{n+1}) \tag{18}$$

converges globally to the exact solution of (17) to first order in Δt.

Proof:
The proof involves two parts. In the first part, we prove consistency. Writing (18) as an algorithm that renders $\mathbf{Y}$ at t_{n+1} as a function of Δt starting from the exact initial condition $\mathbf{Y}(t_n)$.

$$\mathbf{Y}_{n+1}(\Delta t) = \mathbf{Y}(t_n) + \Delta t \mathbf{F}(\mathbf{H}(\mathbf{Y}(t_n)) + \mathbf{e}_n \Delta t,\, \mathbf{Y}_{n+1}). \tag{19}$$

Assuming smoothness of the numerical solution $\mathbf{Y}_{n+1}$ as a function of Δt, and expanding

$$\begin{aligned}
\mathbf{Y}_{n+1}(\Delta t) &= \mathbf{Y}_{n+1}(0) + \Delta t \dot{\mathbf{Y}}_{n+1}(0) + \frac{\Delta t^2}{2!}\ddot{\mathbf{Y}}_{n+1}(0) + \text{h.o.t} \\
&= \mathbf{Y}(t_n) + \Delta t \mathbf{F}(\mathbf{H}(\mathbf{Y}(t_n)),\, \mathbf{Y}(t_n)) \\
&\quad + \Delta t^2(\mathbf{D}_1\mathbf{F}\mathbf{e}_n + \mathbf{D}_2\mathbf{F}\dot{\mathbf{Y}}_{n+1}(0)) + \text{h.o.t.}
\end{aligned} \tag{20}$$

The exact solution at t_{n+1} satisfies the expansion

$$\begin{aligned}
\mathbf{Y}(t_{n+1}) &= \mathbf{Y}(t_n) + \Delta t \dot{\mathbf{Y}}(t_n) + \frac{\Delta t^2}{2!}\ddot{\mathbf{Y}}(t_n) + \text{h.o.t} \\
&= \mathbf{Y}_{n+1}(0) + \Delta t \mathbf{F}(\mathbf{H}(\mathbf{Y}(t_n)),\, \mathbf{Y}(t_n)) \\
&\quad + \frac{\Delta t^2}{2}(\mathbf{D}_1\mathbf{F}\dot{\mathbf{X}} + \mathbf{D}_2\mathbf{F}\dot{\mathbf{Y}}(0)) + \text{h.o.t.}
\end{aligned} \tag{21}$$

Comparing the Taylor series expansion of the exact solution and the numerical scheme for the DAE, we conclude that

$$\|\mathbf{Y}(t_{n+1}) - \mathbf{Y}_{n+1}\| = O(\Delta t^2). \tag{22}$$

The second part of the proof involves exploiting this intermediate result to bound the global error in a standard fashion for stability. In particular, defining $E_{n+1} = \|\mathbf{Y}(t_{n+1}) - \mathbf{Y}_{n+1}\|$, one obtains a recursive relation of the form

$$E_{n+1} \leq \frac{1 + \Delta t L}{1 - \Delta t L} E_n + \delta_n, \tag{23}$$

where δ_n is a term of order $O(\Delta t^2)$ and L is the Lipschitz constant. Solving the recursion relation, one obtains

$$E_{n+1} \leq (1+\alpha)^n E_0 + \delta \frac{(1 - (1+\alpha)^n)}{\alpha} \tag{24}$$

where, $\delta_n \leq \delta$, $\forall n$; and $\alpha = 2\Delta t L/(1 - \Delta t L)$.

Under the limits, $n \to \infty,\ \Delta t \to 0$ and $n\Delta t = T$, it can be inferred that

$$E_{n+1} \leq \exp(n\alpha)E_0 + C\Delta t \frac{1 - \exp(n\alpha)}{2L} \tag{25}$$

for some constant C. In the limit $n \to \infty$, one finally obtains,

$$E_{n+1} \leq \exp(2LT)E_0 + C\Delta t \frac{1 - \exp(2LT)}{2L} \tag{26}$$

which proves the stability of the method.

Remark 3
The conclusions of the above lemma remain true if a higher order ($O(\Delta t^2)$ or more) perturbation is added to the $\mathbf{e}_n \Delta t$ term. □

Remark 4
The split algorithm, $\boldsymbol{\chi}_{2,\Delta t} \circ \boldsymbol{\chi}_{1,\Delta t}$, together with a Backward Euler discretization, exactly corresponds to the timestepping shown in (18) with $\mathbf{e}_n = \mathbf{0}$, thus proving global first order accuracy. □

Remark 5
The fully implicit algorithm, namely,

$$\begin{aligned} \mathbf{G}(\mathbf{X}_{n+1},\ \mathbf{Y}_{n+1}) &= 0 \\ \frac{\mathbf{Y}_{n+1} - \mathbf{Y}_n}{\Delta t} &= \mathbf{F}(\mathbf{X}_{n+1},\ \mathbf{Y}_{n+1}) \end{aligned} \tag{27}$$

is also globally first order accurate, from the following observation. Equations (27) can be rewritten for $\mathbf{Y}_{n+1}$ as,

$$\frac{\mathbf{Y}_{n+1} - \mathbf{Y}_n}{\Delta t} = \mathbf{F}(\mathbf{H}(\mathbf{Y}_{n+1}),\ \mathbf{Y}_{n+1}) \tag{28}$$

and $\mathbf{H}(\mathbf{Y}_{n+1})$ is at worst an $O(\Delta t)$ perturbation of $\mathbf{H}(\mathbf{Y}_n)$ and the lemma above proves first order convergence. The convergence for the fully implicit one step method can also be proved as a special case of a class of Runge-Kutta methods for DAEs (see e.g., Hairer and Wanner [1993]). □

3.5 Order of Accuracy for the Adiabatic Split: Elastic Case

The goal of this section is to prove that the adiabatic split proposed for the spatially discrete equations, is also globally first order accurate. The adiabatic split is implemented with nodal activity $\mathbf{A}$ and nodal displacement $\mathbf{U}$ as the primary variables, while concentration and displacement variables are fixed in each of the phases. In particular, during the mechanical phase, the concentration is fixed point-wise in the interior of the elements, while in the diffusion phase, discrete concentration variables defined below are evolved. Fixing the concentration point-wise in the interior of the elements in the mechanical phase, fixes the discrete weighted-average concentrations. However, displacement evolution in this phase with fixed point-wise concentrations does not lead to the evolution of a C^0 activity field defined through its nodal values. As discussed before, this difficulty is overcome by resorting to sequencing the split phases so that the mechanical phase is ahead of the diffusion phase. In addition a one step, one stage method needs to be used to time-step the diffusion problem. Given the special nature of the split, we note that it is indeed first order convergent. The proof is as follows.
Define the vector of nodal concentrations as:

$$\mathbf{M} = \begin{pmatrix} \int_{\mathbf{\Omega}^e} M(\mathbf{A},\mathbf{U}) N^1 d\mathbf{\Omega} \\ \circ \\ \circ \\ \circ \\ \int_{\mathbf{\Omega}^e} M(\mathbf{A},\mathbf{U}) N^{n_{en}} d\mathbf{\Omega} \end{pmatrix} \tag{29}$$

Further, $\mathbf{M}$ corresponds to the nodes where $\mathbf{A}$ is defined and it is easy to verify that given $\mathbf{U}$, $\mathbf{M} = \mathbf{M}(\mathbf{A})$ is invertible.
From the above observations, although $\mathbf{A}$, and $\mathbf{U}$ are the unknown primary variables, and the activity variables $\mathbf{A}$ evolves in both phases of the split, first order convergence can be proved for $\mathbf{M}$ and $\mathbf{U}$. The proof involves using an auxiliary but formally equivalent splitting algorithm. It is emphasized that the auxiliary splitting algorithm is only used as a formality to effect the proof and not for the implementation.
Consider the following algorithm labeled as ALGO2:

1. Given $\mathbf{U}_n$ and $\mathbf{A}_n$ at time t_n.

2. Calculate $\mathbf{M}_n$ from (29) given $\mathbf{A}_n$ and $\mathbf{U}_n$.

3. **Mechanical Phase:** Find $\tilde{\mathbf{U}}$ by solving (where $\tilde{(\cdot)}$ denotes an intermediate solution)

$$\mathbf{G}(\mathbf{U},\, \tilde{\mathbf{A}}(\mathbf{U},\, \mathbf{M}_n)) = \mathbf{0}. \tag{30}$$

   Equation (30) is consistent with $\dot{\mathbf{M}} = \mathbf{0}$ ($\mathbf{M} = \mathbf{M}_n$), and also defines an intermediate activity field in terms of the nodal unknowns $\tilde{\mathbf{A}}(\tilde{\mathbf{U}}, \mathbf{M}_n)$.

4. **Diffusion Phase:** Fixing $\mathbf{U}$, evolve $\mathbf{M}$ by solving

$$\dot{\mathbf{M}} = \mathbf{F}(\mathbf{U}, \mathbf{M}(\mathbf{U}, \mathbf{A})). \tag{31}$$

   The initial condition is either $\tilde{\mathbf{M}} = \tilde{\mathbf{M}}(\mathbf{U}, \tilde{\mathbf{A}})$ or $\mathbf{M}_n = \mathbf{M}_n(\mathbf{U}_n, \mathbf{A}_n)$, since they are the same. Evolving $\mathbf{M}$ in (31), also equivalently implies evolving $\mathbf{A}$ (with initial conditions $\tilde{\mathbf{A}}$), for fixed $\mathbf{U} = \tilde{\mathbf{U}}$.

5. The variables at time t_{n+1} are obtained as

$$\mathbf{U}_{n+1} = \mathbf{U} \tag{32a}$$
$$\mathbf{A}_{n+1} = \mathbf{A} \tag{32b}$$
$$\mathbf{M}_{n+1} = \mathbf{M}(\mathbf{U}_{n+1}, \mathbf{A}_{n+1}). \tag{32c}$$

Remark 6
From this algorithm, it is clear that although the activity variables evolve in both phases of the splitting algorithm, viewing the algorithm in the variables $\mathbf{M}$ and $\mathbf{U}$, reduces it to the standard form assumed in Section 2, earlier. This simply implies first order convergence for this algorithm. In practice, for evolving the diffusion phase in (31), a one step first order method like explicit or implicit Euler discretization is used. □

The actual implementation of the adiabatic split (labeled earlier as ALGO1), is different from the algorithm, just described. The differences and their implications are discussed below to prove global convergence for ALGO1 as well.

The piecewise continuous concentration field $M(\mathbf{A}, \mathbf{U})$ used in the definition of $\mathbf{M}$, is held fixed during the mechanical phase. This is equivalent to fixing $\mathbf{M}$ during the mechanical phase. The nodal unknowns $\mathbf{U}$ are found by solving

$$\mathbf{G}(\mathbf{U},\, \tilde{\mathbf{A}}(\mathbf{U},\, \mathbf{M}_n)) = \mathbf{0}. \tag{33}$$

In general, solving for $\mathbf{U}$ in (33) need not imply the existence of a C^0 activity field by interpolating nodal activities $\tilde{\mathbf{A}}$, such that $M(\mathbf{A}_n, \mathbf{U}_n) = M(\tilde{\mathbf{A}}, \mathbf{U})$. This brings in difficulty in terms of writing the implementation of the adiabatic split in the standard form for proving convergence. However, we prove pieces that help us take recourse to Lemma 1 for proving convergence.
We relabel the final displacements in ALGO2 and ALGO1 during the mechanical phase as $\mathbf{U}_2$ and $\mathbf{U}_1$, respectively. Correspondingly,

$$\begin{aligned} \mathbf{G}(\mathbf{U}_2,\, \tilde{\mathbf{A}}(\mathbf{U}_2,\, \mathbf{M}_n)) &= \mathbf{0} \\ \mathbf{G}(\mathbf{U}_1,\, \tilde{\mathbf{A}}(\mathbf{U}_n,\, \mathbf{M}_n)) &= \mathbf{0} \end{aligned} \tag{34}$$

implying

$$\mathbf{U}_2 = \Phi(\mathbf{U}_2, \mathbf{M}_n), \text{ and } \mathbf{U}_1 = \Phi(\mathbf{U}_n, \mathbf{M}_n). \tag{35}$$

Expanding,

$$\mathbf{U}_2 = \underbrace{\Phi(\mathbf{U}_n, \mathbf{M}_n)}_{\mathbf{U}_1} + \mathbf{D}_1\Phi.(\mathbf{U}_2 - \mathbf{U}_n) + \text{h.o.t.} \tag{36}$$

Using $\|\mathbf{U}_2 - \mathbf{U}_n\| = O(\Delta t)$, one obtains $\|\mathbf{U}_2 - \mathbf{U}_1\| = O(\Delta t)$. Using the triangle inequality, one obtains $\|\mathbf{U}_1 - \mathbf{U}_n\| \leq \|\mathbf{U}_2 - \mathbf{U}_1\| + \|\mathbf{U}_2 - \mathbf{U}_n\|$ also to be $O(\Delta t)$. In other words, asymptotically, one can write the evolution of the diffusion phase as

$$\dot{\mathbf{M}} = \mathbf{F}(\mathbf{U}_n + \mathbf{e}_n \Delta t, \mathbf{M}). \tag{37}$$

Discretizing, (37) using backward Euler, we are in the situation hypothesized by Lemma 1, thereby proving first order global convergence.

Remark 7
Since the primary variables are activity and displacements, the splitting errors in activity and displacements with respect to the monolithic solution in a time step are only $O(\Delta t)$, although the split solution itself is also globally first order accurate. □

Remark 8
In the viscoelastic case, an additional system of ODEs due to the evolution of the viscoelastic stress at the quadrature points are included. In the deformation phase of the split, one can choose $\dot{q}^{(i)} = 0$ along with $\dot{\mathbf{M}} = \mathbf{0}$, i.e., all the ODE variables are frozen. In the diffusion phase, $q^{(i)}$ evolves with evolving M and frozen u. This is one of a multitude of possible splitting choices and one that generates the canonical DAE form.
The actual implementation of the adiabatic split, however involves the opposite of this, namely, $q^{(i)}$ is frozen in the diffusion phase while it is evolved in the deformation phase, when the field M is frozen. This procedure can be justified as follows. In the deformation phase,

$$\text{Momentum Balance:} \quad \mathbf{S}(\mathbf{A}(\mathbf{M}_n, \mathbf{U}_{n+1}), \mathbf{U}_{n+1}, \mathbf{q}_{n+1}) - \mathbf{s}_{n+1} = \mathbf{0}, \tag{38}$$

$$\text{Viscoelastic Evolution:} \quad \frac{q^{(i)}_{n+1} - q^{(i)}_n}{\Delta t} + \frac{q^{(i)}_{n+1}}{\tau(\mathbf{M}_n,\, \lambda_{n+1})} = \beta \frac{\sigma_p^{\infty} \mid_{t_{n+1}} - \sigma_p^{\infty} \mid_{t_n}}{\Delta t}. \tag{39}$$

Due to the index 1 assumption, $\mathbf{U}$ can be expressed in terms of $\mathbf{q}$ and $\mathbf{M}_n$, via the implicit function theorem. Consequently, $\lambda_{n+1} = \lambda_{n+1}(\mathbf{M}, \mathbf{q}_{n+1})$. As a result, Eqn. (39) takes the form

$$\frac{q^{(i)}_{n+1} - q^{(i)}_n}{\Delta t} = \boldsymbol{\psi}^{(i)}(\mathbf{q}_{n+1}, \mathbf{M}_n), \tag{40}$$

for a suitably defined function $\boldsymbol{\psi}$. Thus after eliminating $\mathbf{U}$, we have a system of ODEs of the form:

$$\dot{q}^{(i)} = \boldsymbol{\psi}^{(i)}(\mathbf{q}, \mathbf{M}) \tag{41}$$

$$\dot{\mathbf{M}} = \mathbf{F}(\mathbf{U}, \mathbf{M}). \tag{42}$$

We can apply an operator split on this system of ODEs, freezing the viscoelastic stresses and concentrations in each of the two phases, respectively. It can be verified that ALGO1 for the visco- elastic case exactly corresponds to this split thereby proving global first order convergence. □

Remark 9
In the 1-D case, both the algorithms mentioned under the Viscoelastic case, render symmetric tangent stiffness for the mechanical problem. However, in higher dimensions, only the former algorithm would provide symmetry while the latter would not. □

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