Finite Element Methods for non-Fickian Polymer Diffusion

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Outline

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The model for non-Fickian diffusion

Problem (Cohen, White & Witelski, 1995)

Find concentration u and stress σ such that

$$\left.\begin{aligned} \dot{u} - D\Delta u - K\Delta\sigma &= 0 \\ \dot{\sigma} + \gamma(u)\sigma &= \mu u \end{aligned}\right\} \quad \text{in domain } \Omega$$

$$u = u_D \qquad \text{on Dirichlet boundary}$$

$$(D\nabla u + K\nabla\sigma)\cdot \boldsymbol{n} = 0 \qquad \text{on Neumann boundary}$$

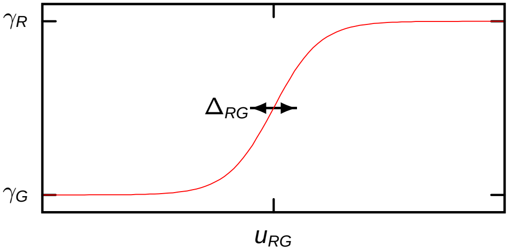
$$\left.\begin{aligned} u(t=0) &= \breve{u} \\ \sigma(t=0) &= \breve{\sigma} \end{aligned}\right\} \quad \text{initial conditions}$$

where $D, K, \mu > 0$ are given constants, u_D, $\breve{u}$, $\breve{\sigma}$ given functions.

Nonlinear Function $\gamma(u)$

- polymers show different behaviour depending on the concentration u: rubbery state, glassy state
- nonlinear function γ models this

$$\gamma(u) := \frac{1}{2}(\gamma_R + \gamma_G) + \frac{1}{2}(\gamma_R - \gamma_G)\tanh\left(\frac{u - u_{RG}}{\Delta_{RG}}\right)$$



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Existence of Solutions

Theorem (Amann, 1991)

For "sufficiently smooth" data and smooth, bounded domain, the problem has a unique solution

$$(u, \sigma) \in C([0, \infty), W_p^2(\Omega, \mathbb{R}^2)) \cap C^1([0, \infty), L_p(\Omega, \mathbb{R}^2)),$$

for any $p \in [2, \infty)$ *with* $p > \dim \Omega$.

- proof uses semigroup theory,
- problem: FE-domain usually not smooth but polygonal

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Discretization

- space discretization: standard FEM,
  - construct mesh with maximum element diameter h,
  - function space W^h: continuous piecewise polynomials,
  - function space V^h: subset of W^h, zero on Dirichlet part of boundary
- time discretization: standard Crank-Nicolson scheme,
  here: constant time-step $k = t_n - t_{n-1}$
  Notation:

$$\partial_t w_n := \frac{w(t_n) - w(t_{n-1})}{k}, \qquad \overline{w}_n := \frac{1}{2}(w(t_n) + w(t_{n-1})).$$

- approximation of nonlinearity $\gamma(u)\sigma$: three methods

Discrete equations

Problem (Discretized formulation)

At each time-step n find $u_n^h \in u_D(t_n) + V^h$ *and* $\sigma_n^h \in W^h$ *such that*

$$
\begin{aligned}
(\partial_t u_n^h, v) + (D\nabla \overline{u}_n^h, \nabla v) &= -(K\nabla \overline{\sigma}_n^h, \nabla v) && \forall v \in V^h,\\
(\partial_t \sigma_n^h, w) + (\mathscr{B}_{n,Q}(u^h, \sigma^h), w) &= (\mu\, \overline{u}_n^h, w) && \forall w \in W^h,
\end{aligned}
$$

- solving at each time-step n using values from previous time-steps
- term $\mathscr{B}_{n,Q}(u^h, \sigma^h)$ that replaces $\overline{\gamma(u^h)\sigma^h}$ will be defined next

Extrapolation for $\gamma(u)$

- We would like to avoid solving nonlinear systems of equations,
- thus extrapolate u^h from previous time-steps, (linearly, except at first time-step $n = 1$):

$$\gamma(u)\Big|_{t_n} \approx \gamma_n^h(\boldsymbol{x}) := \begin{cases} \gamma\left(2u_{n-1}^h(\boldsymbol{x}) - u_{n-2}^h(\boldsymbol{x})\right) & \text{for } n \geq 2 \\ \gamma\left(u_{n-1}^h(\boldsymbol{x})\right) & \text{for } n = 1 \end{cases}$$

$$\gamma(u)\Big|_{t_{n-1/2}} \approx \gamma_n^{\text{half}}(\boldsymbol{x}) := \begin{cases} \gamma\left(\frac{3}{2}u_{n-1}^h(\boldsymbol{x}) - \frac{1}{2}u_{n-2}^h(\boldsymbol{x})\right) & \text{for } n \geq 2 \\ \gamma\left(u_{n-1}^h(\boldsymbol{x})\right) & \text{for } n = 1 \end{cases}$$

Approximation of $\gamma(u)\sigma$

- need to approximate $\overline{\gamma(u^h)\sigma^h} = \frac{1}{2}\gamma(u_n^h)\sigma_n^h + \frac{1}{2}\gamma(u_{n-1}^h)\sigma_{n-1}^h$ to avoid solving nonlinear equations
- replace by $\mathscr{B}_{n,Q}(u^h, \sigma^h)$
- consider three methods $Q \in \{1, 2, 3\}$:

$$\mathscr{B}_{n,1}(u^h, \sigma^h) := \frac{1}{2}\gamma_n^h \sigma_n^h + \frac{1}{2}\gamma(u_{n-1}^h)\sigma_{n-1}^h$$

$$\mathscr{B}_{n,2}(u^h, \sigma^h) := \gamma_n^{\text{half}}\, \overline{\sigma}_n^h$$

$$\mathscr{B}_{n,3}(u^h, \sigma^h) := \frac{1}{2}\sum_{j=1}^{N_\phi} \gamma_n^h(\boldsymbol{x}_j)\sigma_n^h(\boldsymbol{x}_j)\phi_j + \frac{1}{2}\sum_{j=1}^{N_\phi} \gamma(u_{n-1}^h(\boldsymbol{x}_j))\sigma_{n-1}^h(\boldsymbol{x}_j)\phi_j$$

where ϕ_i are Lagrange basis functions and $\boldsymbol{x}_j$ their nodes, i.e. $\phi_i(\boldsymbol{x}_j) = \delta_{ij}$.

Implementation

- All three methods $Q = 1, 2$ and 3 have been implemented for 1D, 2D and 3D using the Alberta FE-library.
- Methods $Q = 1$ and 2 give a combined linear system for u^h and σ^h at each time-step.
- For method $Q = 3$, σ^h can be eliminated from the first equation, giving a smaller linear system.

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Convergence Tests

- Artificial exact solutions can be generated by adding custom forces f and $\hat{f}$:

$$\dot{u} - D\Delta u - K\Delta\sigma = f$$
$$\dot{\sigma} + \gamma(u)\sigma = \mu u + \hat{f}$$

- Numerical evidence suggests that for all three methods

$$\max_n \left\| u(t_n) - u_n^h \right\|_{L_2} + \max_n \left\| \sigma(t_n) - \sigma_n^h \right\|_{L_2} \leq C(h^{r+1} + k^2),$$

where r is the polynomial degree.

Outline

1. The Mathematical Model
   - The Equations
   - Existence and Uniqueness
2. FEM Discretization
   - Discrete Equations
   - Convergence Tests
   - Numerical Examples

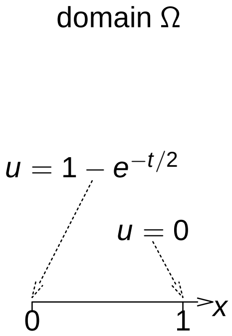
Numerical Examples

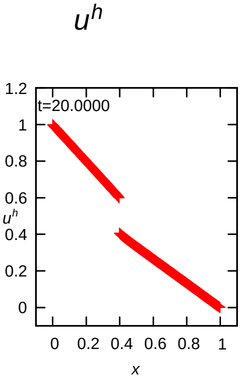
Animations of numerical solutions in 1D, 2D and 3D follow.

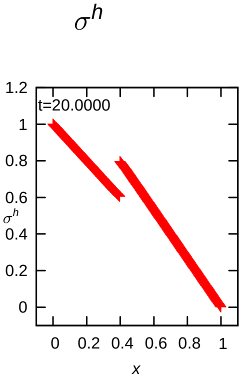
- equation parameters: $D = K = \mu = 1$
- parameters of nonlinear function $\gamma(u)$:
  $\gamma_G = 0.5$, $\gamma_R = 1$, $u_{RG} = 0.5$, $\Delta_{RG} = 0.05$
- Dirichlet boundary conditions at opposite ends of domain, remaining boundary has Neumann conditions

The solution develops a discontinuity in infinite time, as predicted by Cohen, White & Witelski, 1995.

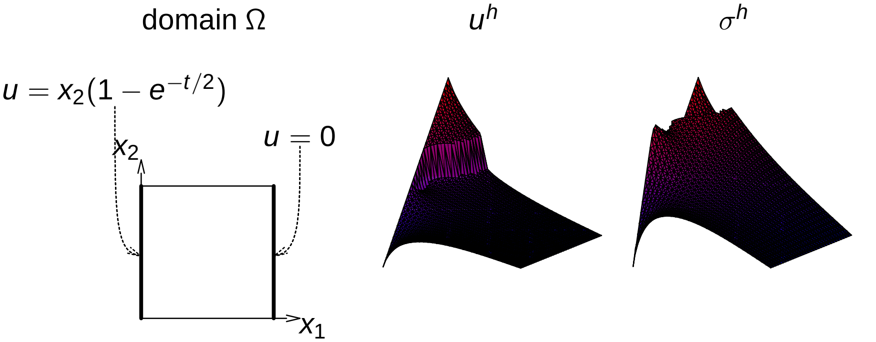
Numerical Example 1D





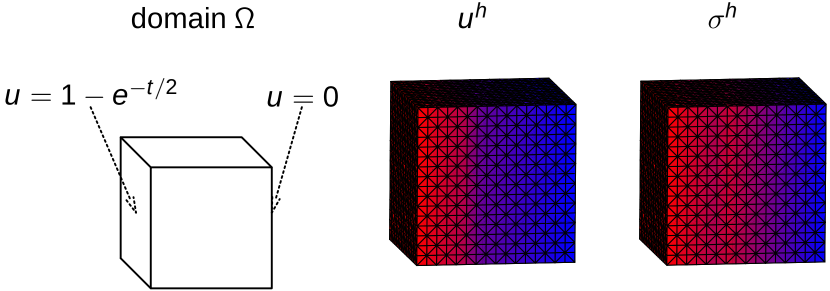


Numerical Example 2D



(graphics: GRAPE)

Numerical Example 3D



(graphics: GRAPE)

Summary

- suggested three methods of discretization for the problem
- methods appear to work in practice

- Outlook
  - aim: derive an *a priori* error estimate to confirm the experimental data, similar to Rivière & Shaw, 2005
  - adaptivity in time and space

For Further Reading

H. AMANN, *Global existence for a class of highly degenerate parabolic systems*, Japan J. Indust. Appl. Math., 8 (1991), pp. 143–151.

D. S. COHEN, A. B. WHITE, AND T. P. WITELSKI, *Shock formation in a multidimensional viscoelastic diffusive system*, SIAM Journal on Applied Mathematics, 55 (1995), pp. 348–368.

B. RIVIÈRE AND S. SHAW, *Discontinuous Galerkin finite element approximation of nonlinear non-Fickian diffusion in viscoelastic polymers*, Technical Report BICOM 05/6, BICOM, Brunel University, London, 2005.

Steady-state with discontinuity I

Cohen, White & Witelski show for certain 2D domains: solution approaches steady-state with discontinuity.
steady-state equations:

$$-D\Delta u - K\Delta\sigma = 0 \quad (1)$$

$$\gamma(u)\sigma = \mu u \quad (2)$$

Using (3) to eliminate σ and setting

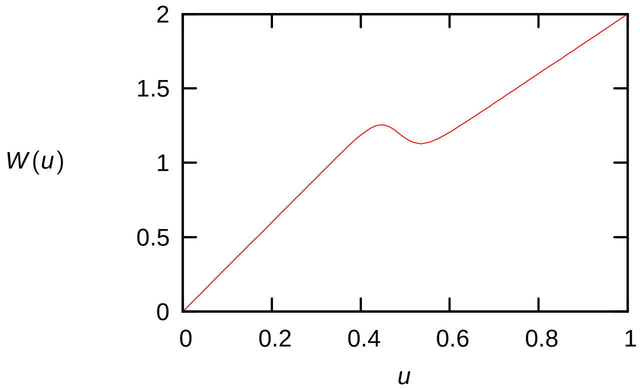
$$W(u) = \left(D + \frac{\mu K}{\gamma(u)}\right)u \quad (3)$$

reduces (1) to

$$-\Delta W(u) = 0$$

Steady-state with discontinuity II

typical shape of W for small enough Δ_{RG}:



$W(u)$ being smooth leads to u being discontinuous.

Convergence Test: Time-Step Size k

$$Q = 1, \text{2D}, u = \cos(t)\sum_i x_i, \quad \sigma = t^3 \sum_i (2-i)x_i.$$

k	error_u	EOC	error_σ	EOC
1.00E+00	1.1803E-01	-	2.3183E-01	-
5.00E-01	3.7672E-02	1.6475	5.5369E-02	2.0659
2.50E-01	9.8629E-03	1.9334	1.2667E-02	2.1280
1.25E-01	2.4955E-03	1.9827	3.2284E-03	1.9722
6.25E-02	6.3417E-04	1.9764	8.1470E-04	1.9865
3.13E-02	1.6011E-04	1.9858	2.0493E-04	1.9911
1.56E-02	4.0238E-05	1.9924	5.1421E-05	1.9947
7.81E-03	1.0087E-05	1.9960	1.2880E-05	1.9972
3.91E-03	2.5255E-06	1.9979	3.2232E-06	1.9986
1.95E-03	6.3182E-07	1.9990	8.0619E-07	1.9993

Convergence Test: Mesh Parameter h

$Q = 3$, 2D, $u = \prod_i \sin(\pi x_i)$, $\quad \sigma = (1-t)\exp(\sum_i x_i)$

polynomial degree 2

DOF	h	error_u	EOC	error_σ	EOC
13	1.00E+00	8.37E-02	-	2.68E-02	-
41	5.00E-01	8.78E-03	3.2526	2.63E-03	3.3517
145	2.50E-01	1.32E-03	2.7303	3.12E-04	3.0712
545	1.25E-01	1.71E-04	2.9511	3.48E-05	3.1648
2113	6.25E-02	2.17E-05	2.9810	3.88E-06	3.1651
8321	3.13E-02	2.74E-06	2.9851	4.81E-07	3.0133
33025	1.56E-02	3.44E-07	2.9933	6.03E-08	2.9959
131585	7.81E-03	4.31E-08	2.9957	7.55E-09	2.9978