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of Concrete**

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Numerical Experiments with Self-Adaptive Finite Element Simulations in 2D for the Carbonation of Concrete

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Abstract

Chemical processes like carbonation of concrete structures are driven by slow diffusion processes and fast reactions. This leads to the formation of relatively sharp reaction fronts, which move slowly through the material. Self-adaptive finite element methods provide a tool to automatically generate meshes locally fine enough to capture the reaction, while coarser meshes are sufficient in the bulk. We demonstrate here the applicability of self-adaptive methods for 2D concrete carbonation problems.

Key words: Adaptive finite element method, reaction-diffusion systems, concrete carbonation, fast reaction

1 Introduction: Need for automatic adaptivity

During carbonation of concrete structures and similar physicochemical processes, relatively sharp reaction fronts move slowly through the material, driven by diffusion processes. In other parts, concentration fields vary only slightly (or not at all).

In order to capture such reaction fronts in a numerical method, a high resolution (equivalent to a fine grid) is needed in those places. But using such a fine grid everywhere, the computation will get very slow, especially in two and three space dimensions. The reason is the stiffness of equations due to high reaction rates, which require stable (and expensive) numerical solution methods and relatively small time steps. On the other hand, such a fine grid is not needed everywhere, because slowly varying concentration fields can easily be approximated on a relatively coarse mesh. Thus, a method which uses a fine mesh near reaction fronts and coarser meshes where possible would make a good balance between accuracy and numerical cost.

Adaptive finite element methods present a tool to automatically give criteria for a local mesh refinement, based on the computed solution (and not only on *a priori* knowledge of an expected behavior). For model problems, even mathematical bounds for the error between approximate and true solution can be shown, as well as quasi-optimality of the meshes generated by the adaptive method. In self-adaptive methods, regions for local refinement

are selected based on local error indicators, which estimate the error contribution of single mesh elements. They are computed from the discrete solution on the current mesh and known data of the problem (like material parameters and boundary values). All mesh elements where these indicators are large must be refined, while elements with very small indicators may even be coarsened. This is important especially for simulations of non-stationary problems, when local internal structures may move or even vanish after some time.

We want to demonstrate here that it is appropriate to apply such self-adaptive finite element methods to a model for the carbonation of concrete in two space dimensions. In the moment, this is only a test for this application, as mathematical proofs for error bounds are not yet derived, and thus error indicators are still purely heuristical. Due to the strong reaction and slow diffusion, it is not even clear what is an appropriate error norm to work with – using the standard L^2 -norm based derivation of adaptive methods would need a Gronwall-like estimate, introducing exponentials of the reaction rate and time scale, which are both large, and thus produce practically irrelevant estimates.

For a survey of durability problems in concrete-based materials, see [5], e.g., and references therein. Specifics on concrete carbonation are subject of [2, 11]. First attempts to deal with 2D carbonation issues (under natural exposure conditions of concrete structures) are published in [1, 7, 10].

2 Concrete carbonation model

For demonstration purposes, we restrict ourselves here to a simple reaction-diffusion model in 2D for the carbonation of concrete, involving the concentrations c_1, c_2 of CO_2 in air and liquid phases, c_3 of $Ca(OH)_2$ in water, and the total moisture concentration c_4 . In a domain $\Omega \subset \mathbb{R}^2$, the carbonation can be modeled by the system of reaction-diffusion equations

$$\partial_t c_1 - D_1 \Delta c_1 = -f^{\text{Henry}}, \quad (1)$$

$$\partial_t c_2 - D_2 \Delta c_2 = f^{\text{Henry}} - f_2^{\text{reac}}, \quad (2)$$

$$\partial_t c_3 - D_3 \Delta c_3 = -f_3^{\text{reac}}, \quad (3)$$

$$\partial_t c_4 - D_4 \Delta c_4 = f_4^{\text{reac}}. \quad (4)$$

Absorption of CO_2 from gaseous to water phase is described by f^{Henry} , while f_i^{reac} denote the productions of species i by the carbonation reaction. This system of equations is completed by appropriate initial values and flux boundary conditions. See [6] for a derivation of this and similar models.

Moving to non-dimensional concentrations $u_i = c_i/c_i^m$ and characteristic time/length scales (compare [6], e.g.), integrating over Ω with a test function v , and integrating the Laplacian by parts, this leads to the weak formulation of (1)-(4) in the Sobolev space $H^1(\Omega)$: For all $v \in H^1(\Omega)$ and times $t \in (0, T)$ holds

$$(\partial_t u_1, v)_\Omega + \delta_1 (\nabla u_1, \nabla v)_\Omega = (-f^{\text{Henry}}, v)_\Omega + W_1^{\text{Rob}}(u_1^{\text{ext}} - u_1, v)_{\partial\Omega}, \quad (5)$$

$$\beta_2(\partial_t u_2, v)_\Omega + \beta_2 \delta_2 (\nabla u_2, \nabla v)_\Omega = (f^{\text{Henry}} - f^{\text{reac}}, v)_\Omega, \quad (6)$$

$$\beta_3(\partial_t u_3, v)_\Omega + \beta_3 \delta_3 (\nabla u_3, \nabla v)_\Omega = (-f^{\text{reac}}, v)_\Omega, \quad (7)$$

$$\beta_4(\partial_t u_4, v)_\Omega + \beta_4 \delta_4 (\nabla u_4, \nabla v)_\Omega = (f^{\text{reac}}, v)_\Omega + W_4^{\text{Rob}}(u_4^{\text{ext}} - u_4, v)_{\partial\Omega}. \quad (8)$$

Here, $(v, w)_G := \int_G vw$ denotes the L^2 -scalar product, and u_i^{ext} is the exterior value giving the flux boundary condition with mass transfer coefficient W_i^{Rob} , which is used here only for gaseous CO_2 and moisture. The system is completed by initial values for u_1, \dots, u_4 at time $t = 0$. They account for the cement chemistry. The absorption and reaction production terms are given by

$$f^{\text{Henry}} = W^{\text{Hen}} \left(\frac{C^{\text{Hen}} u_1}{\phi \phi_a} - \frac{\beta_2 u_2}{\phi \phi_w} \right), \quad f^{\text{reac}} = \Phi^2 F^{\text{Hum}} \frac{u_2^p u_3^q}{(\phi \phi_w)^{p+q-1}},$$

where we denote by ϕ the concrete porosity, ϕ_a, ϕ_w air and water fractions in pores, C^{Hen} the Henry constant, W^{Hen} is an absorption constant, and F^{Hum} is a (constant) humidity factor. The exponents $p, q \geq 1$ are partial reaction orders of the carbonation reaction. Due to the scaling, the previously different reaction production terms now are all the same. The β_i are called impact capacity factors and represent the ratio of the maximum concentration of the i -th species to the maximum $CO_2(g)$ concentration. We denote by δ_i the ratio of the characteristic diffusion time of the $CO_2(g)$ to the characteristic diffusion time of the i -th species. The ratio of the characteristic time for diffusion to the characteristic time for reaction gives the dimensionless coefficient Φ^2 , the Thiele modulus.

3 Finite element approximation

Based on the weak formulation (5)-(8), we derive a finite element method by time discretization and looking for solutions in each time step in a finite dimensional subspace of $H^1(\Omega)$.

Let $0 = t_0 < t_1 < \dots < t_N = T$ define a subdivision of $(0, T)$ into time steps $I_n = (t_{n-1}, t_n)$ with (not necessarily constant) time step sizes $\tau_n = t_n - t_{n-1}$. For each time step, let \mathcal{S}_n be a conforming triangulation of Ω into triangles. Here we assume that the domain has polygonal boundary $\partial\Omega$. Corresponding to these triangulations, we define the spaces X_n of piecewise linear finite element functions $X_n = \{v \in C(\bar{\Omega}) : v|_S \in \mathbb{P}_1(S) \text{ for all } S \in \mathcal{S}_n\}$.

Using an implicit Euler time discretization, we define in every time step the discrete solution $U_1^n, U_2^n, U_3^n, U_4^n \in X_n$, fulfilling for each $V \in X_n$

$$\left(\frac{U_1^n - U_1^{n-1}}{\tau_n}, V \right)_n + \delta_1 (\nabla U_1^n, \nabla V)_\Omega = (-f^{\text{Henry}}, V)_n + W_1^{\text{Rob}}(u_1^{\text{ext}} - U_1^n, V)_{\partial\Omega}, \quad (9)$$

$$\beta_2 \left(\frac{U_2^n - U_2^{n-1}}{\tau_n}, V \right)_n + \beta_2 \delta_2 (\nabla U_2^n, \nabla V)_\Omega = (f^{\text{Henry}} - f^{\text{reac}}, V)_n, \quad (10)$$

$$\beta_3 \left(\frac{U_3^n - U_3^{n-1}}{\tau_n}, V \right)_n + \beta_3 \delta_3 (\nabla U_3^n, \nabla V)_\Omega = (-f^{\text{reac}}, V)_n, \quad (11)$$