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MATHEMATICAL TREATMENT OF DIFFUSION PROCESSES OF GASES AND FLUIDS IN POROUS MEDIA

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Abstract

The transport of fluids and gases in narrow pore systems is described by the transport equation and the material balance equation. Applying the three methods to our parabolic problem shows the advantage that the number of unknowns is dramatically decreased and the implementation of the algorithm on a PC is possible.

Keywords: diffusion processes of gases and fluids.

The transport of fluids and gases in narrow pore systems is described by the transport equation and the material balance equation and leads to the following partial differential equation

$$\frac{\partial c_A}{\partial t} + \frac{\partial a_A}{\partial t} = \operatorname{div}\left(D^{eff} \operatorname{grad} c_A\right), \tag{1}$$

where c_A denotes the concentration of the gas A, a_A the part of the gas A, which is adsorbed, and D^{eff} denotes the diffusion coefficient. If the process is isothermic, we have

$$a_A = f(c_A). \tag{2}$$

So we come to the equation

$$\left(1 + f'(c_A)\right) \frac{\partial c_A}{\partial t} = \operatorname{div}\left(D^{eff} \operatorname{grad} c_A\right), \tag{3}$$

which is a parabolic partial differential equation. At the start of the process we know the concentration from the experiment, which gives us the initial condition

$$c_A = \begin{cases} c_{A,i}, & \text{for } t = 0 \text{ in the interior}, \\ c_{A,R}, & \text{for } t = 0 \text{ on the boundary}. \end{cases} \tag{4}$$

As the first boundary condition we demand that no change of the concentration takes place in the centre of symmetry, say in the origin

$$\text{grad } c_A(0,t) = 0 \quad \text{in the centre of symmetry and for all} \quad t\,. \tag{5}$$

The second boundary condition originates from a balance equation

$$D^{eff} \cdot \text{grad } c_A = -C \cdot \frac{\partial c_A}{\partial t} \qquad \text{on the boundary for all} \quad t\,, \tag{6}$$

where C is a constant with respect to time and space.

Three essential difficulties appear in the system above

1. The differential equation may be nonlinear because the function f in (2) is perhaps nonlinear.
2. The initial condition (4) is not continuous.
3. The boundary conditions are both of Neumann type.

In the first stage we consider the linear part of this initial-boundary-value-problem ($f \equiv 0$) and use the finite element method (FEM). This method is well known and good numerical algorithms are available.

The main idea of the FEM consists in multiplying the equation by a testfunction φ and integrating over the domain Ω. Afterwards we apply the first Green's formula and get the following weak form:

Find $u \in V$ such that for all $\varphi \in V$ we have

$$\int_\Omega \frac{\partial c_A}{\partial t}\varphi \,\mathrm{d}x + \int_\Omega \left(D^{eff}\text{grad } c_A\right) \text{grad } \varphi \,\mathrm{d}x = 0\,. \tag{7}$$

Some difficulties are caused by the non-continuous initial condition. But there are easy ways to replace this condition by a continuous function.

Experiments show that near the boundary where the concentration changes rapidly, we need a very fine grid in order to get satisfactory results. The exact solution seems to have a singularity at the boundary. Theoretical results as in the following theorem confirm this observation for the model problem

Theorem 0.1 *Let $\{\mathcal{T}_h\}$ be a family of regular partitions of Ω where Ω is a polygonal domain, and let V_h be the finite element space.*

(i) If Ω is convex and u_{FE} is the finite element solution of problem (7), then

$$\|u - u_{FE}\|_E \le c \cdot h^\mu \|u\|_{H^k(\Omega)}, \qquad \mu = \min(k-1, p)\,. \tag{8}$$

(ii) If Ω is non-convex, then for fixed $\varepsilon > 0$:

$$\|u - u_{FE}\|_E \leq c(\varepsilon) \cdot h^{\pi/\alpha_m - \varepsilon} \|u\|_{H^{2,t}} . \tag{9}$$

(iii) If Ω is non-convex and $f \in L_2(\Omega)$ then

$$\|u - u_{FE}\| \leq c \cdot h^{2\pi/\alpha_m - \varepsilon} \|f\| . \tag{10}$$

The norm with index 'E' signifies the energy norm, which is here the H^1-norm. $H^{2,t}$ is the weighted Sobolev space with the norm given by

$$|u|_{2,\Omega,t} := \sum_{|\beta|=2} \int_\Omega \varrho^t \left(D^\beta u\right)^2 \mathrm{d}x , \qquad \varrho \text{ the distance to } 0 . \tag{11}$$

The so-called Shift Theorem explains the lack of continuity in the exact solution of our model problem

$$\begin{aligned} -\Delta u &= f \quad \text{in} \quad \Omega , \\ u &= 0 \quad \text{on} \quad \partial\Omega . \end{aligned} \tag{12}$$

Theorem 0.2 (Shift Theorem) *Let $u \in H_0^1(\Omega)$ be the solution of (7).*

(i) If Ω has C^k-boundary $\partial\Omega$, $k \geq 2$ and *$f \in H^{k+2}(\Omega)$*, then:

$$u \in H^k(\Omega) \qquad \textit{and} \qquad \|u\|_{k,\Omega} \leq C \cdot \|f\|_{k-2,\Omega} . \tag{13}$$

(ii) If Ω is convex, $f \in L_2(\Omega)$ then:

$$u \in H^2(\Omega) \qquad \textit{and} \qquad \|u\|_{2,\Omega} \leq C \cdot \|f\|_\Omega . \tag{14}$$

(iii) If Ω is a non-convex polygonal domain with interior angles $0 < \alpha_1 \leq \alpha_2 \leq \ldots \leq \alpha_{m-1} < \pi$, $\pi < \alpha_m \leq 2\pi$ (this vertex at the origin), $f \in L_2(\Omega)$, then:

$$u \in H^{1+k-\varepsilon}(\Omega), \qquad k = \frac{\pi}{\alpha_m} , \qquad \|u\|_1 + \|u\|_{2,t} \leq C_t \cdot \|f\|_\Omega$$

$$\textit{for any} \quad t > 2\left(1 - \frac{\pi}{\alpha_m}\right) . \tag{15}$$

Therefore it is natural to refine the triangulation close to the boundary in order to increase the accuracy. Here a geometric mesh seems to be useful.

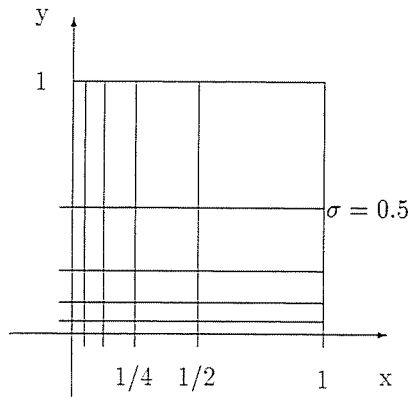

Fig. 1. Geometric mesh

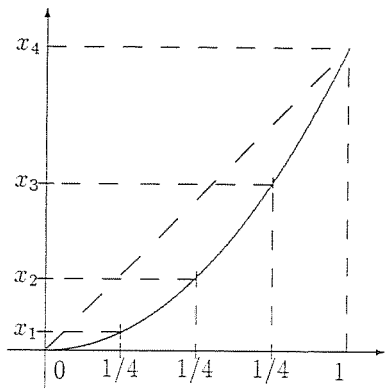

Fig. 2. Graded mesh

With a given parameter σ with $0 < \sigma < 1$ and a rectangle $0 \leq x \leq 1$, $0 \leq y \leq 1$, we consider the net generated from the lines

$$x_0 = 0\,, \quad x_i = \sigma^{n-i}\,, \quad y_0 = 0\,, \quad y_j = \sigma^{n-j}\,, \quad i, j = 1, \ldots, n\,. \tag{16}$$

Fig. 1 gives a short impression for $\sigma = 0.5$, $n = 5$.

Another possibility lies in a graded mesh. There the gridpoints are chosen with the help of a function $g(x) = x^{\beta}$, $\beta > 0$. The following figure shows how to choose the meshpoints in each direction.

In general the behaviour of the exact solution is not known beforehand and it is not clear where to refine the finite element mesh locally. The

mathematical answer is a method for automatic mesh refinement, a so-called adaptive method.

In 1981 I. BABUŠKA and A. MILLER proposed in a pioneering work the first adaptive method regarding the one dimensional problem

$$-\frac{\mathrm{d}}{\mathrm{d}x}\left(a(x)\frac{\mathrm{d}u}{\mathrm{d}x}\right) = f(x), \qquad u(0) = u(1) = 0\,. \tag{17}$$

The error estimate at each step is based on solving local problems involving a local residual, and the refinements are carried out according to the size of the solutions of the local problems.

With the error estimator

$$\eta_i := \frac{1}{\sqrt{12}} \cdot \frac{h_i}{\sqrt{a_{i+1/2}}} \cdot \|r_i\|\,, \tag{18}$$

where r_i is the residuum and $a_{i+1/2}$ the value of the coefficient function at the midpoint of the subinterval, they defined the global error estimator

$$\varepsilon(\eta) := \left[\sum_{i=1}^{m}(\eta_i)^2\right]^{\frac{1}{2}}, \tag{19}$$

and gave the following *Adaptive Algorithm* Given tolerance $\delta > 0$.

1. Choose an initial uniform mesh Δ_h.
2. Compute the corrresponding FE-solution.
3. Compute the global error estimator via residuum.
4. If $\varepsilon \leq \delta$, then stop and accept the FE-solution.

If not, refine the mesh to fulfil the inequality. K. ERIKSSON and C. JOHNSON followed in 1988 with an approach different from the BABUŠKA method. Their error control is based on an optimal a priori estimate. They introduced the difference operator

$$D_H^{\gamma}(v(x)) = \frac{v(x \pm \gamma H) - v(x)}{H}, \qquad \gamma = (1,0) \quad \text{or} \quad \gamma = (0,1)\,, \tag{20}$$

and computed for each $x \in K \in T_h$

$$D_H^2(u_h(x)) := \max\left\{|D_H^{\gamma} D^{\alpha} u_h(y)| : |\alpha| = |\gamma| = 1\,, |y - x| \leq C\underline{h}\right\}, \tag{21}$$

with $\underline{h} = \min_{K \in T_h} h_K$. If then for all $K \in T_h$

$$C_0 h_K D_H^2(u_h; K) \leq \delta, \qquad \text{with} \qquad D_H^2(u_h; K) := \max_{x \in K} D_H^2 u_h(x), \tag{22}$$

then stop and accept the solution. If not, refine the mesh to fulfil the inequality.

ASADZADEH and ERIKSSON (1991) gave a different adaptive algorithm for the model problem

$$\Delta u = 0 \qquad \text{in} \quad \Omega^c := \mathbb{R} \backslash \overline{\Omega}, \tag{23}$$

$$\frac{\partial u}{\partial n} = g \qquad \text{on} \quad \Gamma. \tag{24}$$

They transformed the differential equation in an integral equation of the second type

$$\varphi(x) - T\varphi(x) := \varphi(x) - \frac{1}{2\pi} \int_\Gamma \varphi(y) \frac{\partial}{\partial n_x} \log \frac{1}{|x-y|} \mathrm{d}\Gamma_y = -2g(x), \quad x \in \Gamma, \tag{25}$$

and proposed to fix some element $x \in \mathbb{R}^2$ and to compute the residuum

$$r_h^i(y) := \varphi_h^i(y) - T\varphi_h^i(y) + 2g(y). \tag{26}$$

If

$$h_K \leq \frac{\delta 16\pi^2}{CN} \inf_{y \in K} \frac{|x-y|^{\frac{1}{2}}}{|r_h^i(y)|} \qquad \text{for all} \qquad K \in T_h, \tag{27}$$

then stop and accept the solution. If not, refine all the elements K where the inequality is violated.

Applying the three methods to our parabolic problem shows the advantage that the number of unknowns is dramatically decreased and the implementation of the algorithm on a PC is possible.

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