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ADAPTIVE FINITE ELEMENTS FOR VISCOELASTIC FLOWS (ECCOMAS CFD 2010)

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Abstract. *We present some applications of adaptive finite element methods to viscoelastic flow problems arising from the modeling of polymer liquids. As an example we consider the Giesekus model. Our special interest is in error estimators either related to the prediction of certain energy functionals from the continuous model or to independent physical quantities as the drag coefficient or the flow rate through an orifice.*

The flow equations are discretized by a nonconforming finite element method, for which we have shown the preservation of positivity of the conformation tensor. We employ a Newton-type iteration with solution of the linear subproblems by a multigrid solver.

The a posteriori error estimation for nonconforming finite element methods requires special care, already in the case of linear elliptic equations. From a theoretical point of view, the nonconformity implies the loss of orthogonality. By a careful analysis, this difficulty can be surmounted and we have recently proven the quasi-optimality of the method for the Laplace and Stokes equations. Here, the term quasi-optimality refers to the speed of decrease of the error with respect to the number of mesh cells.

In this talk we are interested in the computation of the drag coefficient of an immersed body in a polymer liquid. In order to do so, we derive an a posteriori error estimator, which is used in an adaptive mesh refinement algorithm.

1 INTRODUCTION

Viscoelastic liquids are characterized by a memory effect and an intermediate behavior between a viscous liquid and an elastic solid. Moreover, they are non-Newtonian fluids. Their non- Newtonian behavior can be seen in a variety of physical phenomena, which cannot be predicted by the Navier-Stokes equations. Despite the numerous efforts, the numerical approximation of viscoelastic flows is still a challenging research area, due to their intrinsic properties and to the internal coupling between the viscoelasticity of the liquid and the flow, which is quantified by the Weissenberg number We.

Our contribution is devoted to the computation of the drag coefficient in a polymer flow, which is a classical problem in the field. We propose to use local mesh refinement directly intended to approximate the physical quantity, which is considered as a functional on the approximation space (goal-oriented error estimation). Following the approach of [2], we introduce an adjoint problem, the solution of which is intended to measure the influence of local residuals on the accuracy of the computed functional.

2 MODELING OF POLYMER LIQUIDS

We consider the flow of the polymer liquid described by the following system of equations, known as the Giesekus model [5] involving the velocity field v, pressure p and stress-field τ with assumed constant density ρ, viscosity μ:

$$\rho\left(v_t + v\cdot\nabla v\right) - \operatorname{div}\,\tau + \nabla p = 0, \tag{1}$$

$$\operatorname{div}\,v = 0, \tag{2}$$

$$\tau + \lambda\left(\tau_t + v\cdot\nabla\tau - \nabla v\tau - \tau\nabla v^T\right) + \tilde{\alpha}\tau^2 = 2\mu D(v). \tag{3}$$

The last equation (3) is the constitutive equation relating the stress-field τ to the strain-tensor $D(v)$, involving the relaxation time λ as well as the parameter $\tilde{\alpha}$. The system has to be completed by appropriate initial and boundary conditions, which is in general a difficult task.

In the present study, we are interested in permanent flows, $v_t = \tau_t = 0$. Therefore a variational formulation of (1-3) reads: Find $u = (v, p, \tau) \in (v_d, 0, \tau_d) + U$ such that for all $\delta u = (\delta v, \delta p, \delta\tau) \in U$

$$\langle \rho v\cdot\nabla v, \delta v\rangle + \langle \tau, D(v)\rangle - \langle p, \operatorname{div}\,\delta v\rangle = 0 \tag{4}$$

$$\langle \operatorname{div}\,v, \delta p\rangle = 0 \tag{5}$$

$$\langle \tau + \lambda\left(v\cdot\nabla\tau - \nabla v\tau - \tau\nabla v^T\right) + \tilde{\alpha}\tau^2, \delta\tau\rangle = 2\langle \mu D(v), \delta\tau\rangle. \tag{6}$$

The space U and the vector v_d and tensor τ_d incorporate non-homogenuous Dirichlet boundary conditions (τ_d is prescribed on the inflow boundary $v\cdot n < 0$). The natural boundary conditions implied by (4-6) are $\sigma n = 0$ with $\sigma = \tau - pI$. We write (4-6) in short form as: Find $u \in u_d + U$ such that for all $\delta u \in U$

$$a(u)(\delta u) = 0. \tag{7}$$

The considered finite element discretization of (1-3) is based on a nonconforming velocity space as well as piecewise-constant approximations of p and τ (the symmetry of τ is built in directly). We denote by $\mathcal{H}$ a family of locally refined meshes, starting with an initial mesh h_0. A mesh smoothness condition is imposed in $\mathcal{H}$ which avoids multiple layers of hanging nodes. For given $h \in \mathcal{H}$ we denote by U_h the finite element approximation of U. Assuming for simplicity that v_d and τ_d can be represented by the finite element spaces without error, the discrete system reads: Find $u_h = (v_h, p_h, \tau_h) \in (v_d, 0, \tau_d) + U_h$ such that for all $\delta u_h = (\delta v_h, \delta p_h, \delta\tau_h) \in U_h$

$$\langle \rho v_h \cdot \nabla v_h, \delta v_h\rangle + s_h(v_h, \delta v_h) + \langle \tau_h, D(v_h)\rangle - \langle p_h, \mathrm{div}\ \delta v_h\rangle = 0 \tag{8}$$

$$\langle \mathrm{div}\ v_h, \delta p_h\rangle = 0 \tag{9}$$

$$\lambda t_h(v_h, \tau_h, \delta\tau_h) + \langle \tau_h - \lambda\left(\nabla v_h \tau_h + \tau_h \nabla v_h^T\right) + \tilde{\alpha}\tau_h^2, \delta\tau_h\rangle = 2\langle \mu D(v_h), \delta\tau_h\rangle, \tag{10}$$

where s_h is a bilinear form needed to recover the Korn inequality for nonconforming spaces,

$$s_h(v_h, \delta v_h) := -\sum_{S\in\mathcal{S}_h} \frac{\gamma}{|S|}\int_S [\pi_S^1 v_h \cdot n][\pi_S^1 \delta v_h \cdot n]\, ds + \sum_{K\in\mathcal{K}_h} \beta(D(v_h) - \pi_K^0 D(v_h))(D(\delta v_h) - \pi_K^0 D(\delta v_h))\, dx, \tag{11}$$

defined on the edges $\mathcal{S}_h$ and cells $\mathcal{K}_h$ of the mesh h, involving the local $L^2(A)$-projections π_A^k on polynomials of order k, $A = S$ or $A = K$, and t_h is the Lesaint-Raviart upwind form defined by

$$t_h(v_h, \tau_h, \delta\tau_h) := \sum_{S\in\mathcal{S}_h} \int_S [\tau_h]((v_h \cdot n_S)^+ \delta\tau_h^{ex} + (v_h \cdot n_S)^- \delta\tau_h^{in})\, ds. \tag{12}$$

Here $\tau_h^{in/ex}$ denote the inward/outward value of the discontinuous function τ_h on a given edge S, depending on the chosen normal n_S, and $[\tau_h] = \tau_h^{in} - \tau_h^{ex}$ for an internal edge, whereas $[\tau_h] = \tau_h^{in} - \tau_d$ for a boundary edge.

The short form of (8-10) reads: Find $u_h \in u_d + U$ such that for all $\delta u \in U_h$

$$a_h(u_h)(\delta u_h) = 0. \tag{13}$$

3 COMPUTATION OF THE DRAG COEFFICIENT

Let as assume that we wish to compute the drag coefficient on an immersed object with boundary $\Gamma \subset \partial\Omega$. It is defined (up to a multiplicative constant) as the mean forces projected in a given direction $q \in \mathbb{R}^2$:

$$J(u) := \int_\Gamma n^T \sigma q\, ds. \tag{14}$$

It is well known that the direct computation of the drag coefficient, $J(u_h)$ only yields first-order convergence. A better approach [6] is based on the fact that (14) is related to the natural boundary conditions. Indeed, integration by parts shows that for arbitrary w

$$\langle \rho v \cdot \nabla v, w\rangle + \langle \sigma, D(w)\rangle = \langle \underbrace{\rho v \cdot \nabla v - \mathrm{div}\ \sigma}_{=0}, w\rangle + J(u).$$

Therefore, it is proposed to compute instead

$$J_h^{w_h} := \langle \rho v_h \cdot \nabla v_h, w_h\rangle + s_h(v_h, w_h) + \langle \sigma_h, D(w_h)\rangle, \tag{15}$$

where w_h is a discrete function satisfying $w_h|_\Gamma = q$ and $w_h|_{\partial\Omega\setminus\Gamma} = 0$.

First, we notice that $J_h^{w_h}$ does not depend on the choice of w_h satisfying the indicated boundary conditions. Indeed, let w_h^1 and w_h^2 two such vectors. Then $\delta w_h := w_h^1 - w_h^2 \in U_h$ can be used as a test function in (8) leading to $J_h^{w_h^1} = J_h^{w_h^2}$, and we may suppress the superscript in the following.

The improved accuracy is explained as follows. First we note that with $z_h := (w_h, 0, 0)$ we have

$$J = a_h(u)(z_h) \quad \text{and} \quad J_h = a_h(u_h)(z_h),$$

such that with $\tilde{a}_h(u_1, u_2)(\delta u, z) := \int_0^1 a_h'(su_1 + (1-s)u_2)(\delta u, z)\, ds$

$$J - J_h = \tilde{a}_h(u, u_h)(u - u_h, z_h)$$

We are now lead to the introduction of the adjoint problem: Find $z \in (q, 0, 0) + U$ such that for all $\delta u \in U$

$$a'(u)(\delta u, z) = 0. \tag{16}$$

Since $a'(u)(\delta u, z) = a_h'(u)(\delta u, z)$ it follows that

$$J - J_h = a_h'(u)(u - u_h, z_h - z) + \text{HOT}.$$

Since z_h can be chosen arbitrary (but respecting the boundary conditions), we can take it as a (nonconforming) finite element interpolation of z, and this explains the second-order behavior of the method.

4 A POSTERIORI ERROR ESTIMATION

The adjoint problem (16) plays a crucial role in our a posteriori error estimator, since it allows us to relate the classical local residual terms to the drag functional. It is therefore interesting to have a closer look at its structure. With $z = (w, r, \xi)$ the linear system (16) reads in operator form:

$$\rho\left(-v\cdot\nabla w + \nabla v^T w\right) + 2\mu\,\text{div}\;\xi + L(\tau)\xi - \nabla r = 0, \tag{17}$$

$$-\text{div}\; w = 0, \tag{18}$$

$$\xi + \lambda\left(-v\cdot\nabla\xi - \nabla v\,\xi - \xi\,\nabla v^T\right) + \tilde{\alpha}\tau\xi = D(w), \tag{19}$$

where $L(\tau)\xi := \text{div}\;(\xi\tau^T + \tau^T\xi) + \nabla\tau : \xi$.

The boundary conditions for (17-19) are implied by its weak formulation (16). It can be seen that the transport operators have opposite sign, as compared to the direct problem. In addition, several terms arise from the different nonlinearities of (1-3).

In our algorithm, we propose to discretize the adjoint system (17-19) on the same mesh h as (8-10). Formally, we define $z_h \in (q, 0, 0) + U$ to be the solution of

$$a'(u_h)(\delta u_h, z_h) = 0 \quad \forall \delta u_h \in U_h. \tag{20}$$

We next define quantities $\eta_h = \eta_h(u_h)$ and $\zeta_h = \zeta_h(u_h, z_h)$ such that

$$|J - J_h| \leq C\,\eta_h(u_h)\,\zeta_h(u_h, z_h) + \text{HOT}.$$

Following classical a posteriori error estimators for the nonconforming discretization of the Stokes equation, see for example [4], we define

$$\begin{aligned}\eta_h^2 \;:=\; & \sum_{S\in\mathcal{S}_h} |S|^{-1}\|[v_h]\|_S^2 + \sum_{K\in\mathcal{K}_h} |K|\,\|v_h\cdot\nabla v_h\|_K^2 \\ & + \sum_{S\in\mathcal{S}_h} \||v_h\cdot n|^{1/2}[\tau_h]\|_S^2 + \sum_{K\in\mathcal{K}_h} |K|^{1/2}\|\tau_h - \lambda\left(\nabla v_h\tau_h + \tau_h\nabla v_h^T\right) + \tilde{\alpha}\tau_h^2 - 2\mu\, D(v_h)\|_K^2\end{aligned} \tag{21}$$

and

$$\begin{aligned}\zeta_h^2 \;:=\; & \sum_{S\in\mathcal{S}_h} |S|^{-1}\|[w_h]\|_S^2 + \sum_{K\in\mathcal{K}_h} |K|\,\|v_h\cdot\nabla w_h\|_K^2 \\ & + \sum_{S\in\mathcal{S}_h} \||v_h\cdot n|^{1/2}[\xi_h]\|_S^2 + \sum_{K\in\mathcal{K}_h} |K|^{1/2}\|\xi_h - \lambda\left(\nabla v_h\xi_h + \xi_h\nabla v_h^T\right) + 2\tilde{\alpha}\tau_h\xi_h^2 - D(w_h)\|_K^2\end{aligned} \tag{22}$$

5 ADAPTIVE ALGORITHM

We suppose to have a local mesh refinement algorithm $\mathbb{REF}(h, \mathcal{M})$ which, for given $h \in \mathcal{H}$ and $\mathcal{M} \subset \mathcal{K}_h$, produces a new mesh $h' \in \mathcal{H}$ such that at least all cells in $\mathcal{M}$ are refined. In general, additional cells $K \notin \mathcal{M}$ will be refined in order to meat certain mesh smoothness criteria. For the complexity analysis, it is crucial that the number of additionally refined cells can be controlled by the set of marked cells. This is general not possible to be done in one step, but for some algorithms it can be controlled with respect to the number of the marked cells in previous steps, see [3] for details in the case of the new vertex bisection algorithm.

The adaptive algorithm is given next.

Goal-oriented AFEM

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1. (Initialization) Choose an initial mesh h_0, and set $n = 0$.
2. (Solve) Solve the discrete problems on mesh h_n with solution u_{h_n} and z_{h_n}.
3. (Estimate) Compute the terms of the error estimators $(\eta_h(K))_K$ and $(\zeta_h(K))_K$.
4. (Mark) Define a set $\mathcal{M}_n \subset \mathcal{K}_{h_n}$ of marked cells.
5. (Refine)$h_{n+1} := \mathbb{REF}(h_n, \mathcal{M}_n)$, set $n := n + 1$ and go to step(Solve).

The crucial step is (Mark). Let us denote $h := h_n$. We follow [1] and define a weighted estimator as follows: Let ξ_h be defined as the following weighted estimator

$$\xi_h^2(K) := \frac{\zeta_h^2}{\eta_h^2 + \zeta_h^2}\eta_h^2(K) + \frac{\eta_h^2}{\eta_h^2 + \zeta_h^2}\zeta_h^2(K) \tag{23}$$

Then define $\mathcal{M}_n$ to be a solution to the discrete optimization problem

$$\inf_{\mathcal{M}\in\mathbb{M}_n} \#\mathcal{M}, \quad \mathbb{M}_n := \left\{ \mathcal{M} \subset \mathcal{K}_h : \sum_{K\in\mathcal{M}} \xi_{h_n}^2(K) \geq \theta\, \xi_h^2 \right\}. \tag{24}$$

(24) is the classical bulk criterion known from adaptive finite element algorithms for control of the energy in elliptic equations. The weighting implies that more importance will be given to one of the residuals if they are not balanced.

6 CONCLUSIONS

We have presented a way to goal-oriented adaptivity for viscoelastic flows. At hand of the computation of the drag coefficient of a body in a polymer liquid, we have exhibited an adjoint equation, which relates the classical local residual terms to the error in functional.

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