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Report on the Doctoral Thesis

Finite Element Approximation of Problems in Non-Newtonian Fluid Mechanics

submitted by Dipl.-Math. Adrian Hirn

The present thesis deals with the numerical analysis of certain mathematical models for describing non-Newtonian flow behavior such as "shear thinning" or "shear thickening". Such phenomena frequently occur, e.g., in hemodynamics, lubrication and geophysics, and their quantitative description is of high practical importance. Presently the theoretical analysis of these models as well as their numerical simulation is far from being satisfactorily understood.

The basic model is that of the classical (isothermal) Navier-Stokes equations

$$\rho\partial_t \mathrm{v} + \rho(\mathrm{v}\cdot\nabla)\mathrm{v} - \nabla\cdot\mathcal{T} = \rho \mathrm{f}, \quad \nabla\cdot\mathrm{v} = 0,$$

for an "incompressible" Stokes fluid with the generalized Cauchy stress tensor

$$\mathcal{T} = -\mu\mathcal{I} + \mathcal{S}(\pi, |\mathcal{D}|^2), \quad \mathcal{D} = \tfrac{1}{2}(\nabla\mathrm{v} + \nabla\mathrm{v}^T).$$

Important examples for the extra stress tensor $\mathcal{S} = \mathcal{S}(\pi, |\mathcal{D}|^2)$ are the so-called "power-law model" and the "Carreau model", involving only shear-stress dependence,

$$\mathcal{S}(|\mathcal{D}|^2) = \mu_0|\mathcal{D}|^{p-2}\mathcal{D}, \quad \mathcal{S}(|\mathcal{D}|^2) = \mu_0\big(\epsilon^2 + |\mathcal{D}|^2\big)^{(p-2)/2}\mathcal{D},$$

with fluid-dependent parameters $\mu_0 > 0$, $p \in (1,\infty)$, and $\epsilon > 0$. These models are generally referred to as "p-Stokes" or "p-Navier-Stokes" equations reflecting the nonlinear dependence of the viscosity on the shear tensor. Other considered models involve also a mild (sublinear) dependence of the viscosity on the pressure such as for example

$$\mathcal{S}(\pi, |\mathcal{D}|^2) = \mu_0\big(\epsilon^2 + (\delta + \exp(\alpha\pi))^{-s} + |\mathcal{D}|^2\big)^{(p-2)/2}\mathcal{D},$$

with fluid-dependent parameters $s, \alpha, \epsilon, \delta \geq 0$. The treatment of superlinear dependence of the form $\mathcal{S}(\pi) \approx \exp(\alpha\pi)$ as commonly considered in practical applications (e.g. in lubrication) is still an open problem. The theory and numerical analysis of the standard Newtonian case, case $p = 2$, is already well developed in the literature. Also the numerical analysis, especially the finite element Galerkin approximation, of the simpler "p-Laplace equation" is well understood. In this context the main goals of the present thesis are:

- Extension of the commonly used finite element approximations for the classical Navier-Stokes equations (case $p = 2$) on the one hand and the p-Laplace equation on the other hand to the (incompressible) p-Navier-Stokes equations. This especially includes the design of appropriate (nonlinear) stabilization of the pressure gradient in case of "equal-order" pairs $\mathbf{H}_h \times L_h$ of finite element spaces for velocity and pressure for circumventing the so-called "inf-sup stability" condition,

$$\inf_{\pi_h\in L_h}\sup_{\mathrm{v}_h\in\mathbf{H}_h}\frac{(\pi_h, \nabla\cdot\mathrm{v}_h}{\|\pi_h\|\|\nabla\mathrm{v}_h\|} \geq \gamma > 0.$$

- Derivation of a priori error estimates for these approximations,

$$\|\mathrm{v} - \mathrm{v}_h\| = \mathcal{O}(h^?), \quad \|\pi - \pi_h\| = \mathcal{O}(h^?),$$

which are order-optimal and only use the natural degree of regularity to be expected for the solutions.

- Design of appropriate transport stabilization based on multi-scale concepts for the p-Navier-Stokes equations, which preserves the natural orders of convergence known from the case $p = 2$.

- Derivation of "goal-oriented" a posteriori error representations of the form

$$J(\mathrm{v}, \pi) - J(\mathrm{v}_h, \pi_h) \approx \sum_{T \in \mathcal{T}_h} \rho_T(\mathrm{v}_h, \pi_h)\omega_T(\tilde{\mathrm{z}}_h),$$

and corresponding mesh adaptation strategies for the (nonlinear) p-Navier-Stokes equations using the Dual Weighted Residual (DWR) approach.

- Numerical analysis of the limit case of the "singular" power-law system

$$\mathcal{S}(|\mathcal{D}|^2) = \mu_0 |\mathcal{D}|^{p-2}\mathcal{D}, \quad p \in (1, 2),$$

which leads to unbounded viscosity for vanishing shear stress. In this case linearization and consequently the convergence of the Newton iteration is a delicate matter.

- Inclusion of certain models of pressure-dependent viscosity.

- Treatment of other boundary conditions besides the usual "no-slip" condition,

$$\mathrm{v}|_{\Gamma_{\mathrm{in}}} = \mathrm{v}_{\mathrm{in}}, \quad \mathrm{v}|_{\Gamma_{\mathrm{rigid}}} = 0, \quad -\tfrac{1}{2}\mu(|\mathcal{D}\mathrm{v}|^2)\partial_n \mathrm{v} + \pi \mathrm{n} = P\mathrm{n},$$

for describing nonhomogeneous in- and "free" outflow (so-called "do nothing" outflow boundary condition) in order to apply the developed results to well established pipe flow benchmarks.

In the seven main chapters of this thesis complete answers are given to most of these questions.

Following the brief introduction (Chapter 1) in Chapter 2 some basic results are recalled from the literature on the variational formulation and well-posedness of the p-Stokes and p-Navier-Stokes equations for incompressible fluids. This provides the theoretical basis of the finite element analysis of this problem, which is the main theme of this thesis. Also models with pressure dependent viscosity are discussed. The structural assumptions on the extra stress tensor are formulated in a general manner in order to abstract from the concrete situations considered in the numerical examples.

The standard finite element discretization of the p-Navier-Stokes equation is described in Chapter 3. Here, so-called spaces of "equal-order" shape functions are considered for velocity and pressure, which do not satisfy the usual "inf-sup" stability condition. This lack of stability is circumvented by certain stabilization procedures such as the SUPG stabilization of Hughes et al. or the LPS method of Becker & Braack. Both approaches can also be used for stabilizing dominant transport. As basis for the following a priori error analysis besides the standard interpolation error estimates in Sobolev spaces also some non-standard estimates in Orlicz-Sobolev spaces are recalled from the literature. The chapter closes with the description of the details of the practical realization of these methods within the software package Gascoigne. The linearization of the nonlinear discrete problems is by a Newton iteration with standard step size control.

The linear subproblems are solved by the Generalized Minimal Residual Method (GMRES) with multigrid preconditioning using a block-ILU iteration of "Vanka-type" for smoothing. All these algorithmic ingredients are already well established in the literature. A first series of numerical tests demonstrates the orders of convergence recalled from the literature for various values of the model parameter p. This test also confirms the correctness of the numerical code.

Chapter 4 deals with the finite element approximation of the stationary as well as the nonstationary p-Stokes equations. It contains the main results of this thesis formulated in Theorems 4.11 and 4.12. As "equal-order" elements are used for velocity and pressure stabilization of the pressure gradient is necessary. This is achieved by the "Local Projection Stabilization (LPS)" of Becker & Braack, which is adjusted here to the p-structure of the problem. The proposed (nonlinear) modification of the LPS provides control of a weighted $L^{p'}$-norm, $p' = p/(p-1)$, of the pressure gradient and coincides with the usual LPS for $p = 2$. A careful error analysis shows that, in general, the traditional LPS only yields suboptimal (in fact dimension-dependent) approximation behavior, while the new p-LPS allows to prove optimal-order error estimates, at least for $p \in (1,2]$,

$$\|\mathcal{F}(\mathcal{D}\mathrm{v}) - \mathcal{F}(\mathcal{D}\mathrm{v}_h)\|_{L^2} = \mathcal{O}(h), \quad \|\mathrm{v} - \mathrm{v}_h\|_{W^{1,p}} = \mathcal{O}(h), \quad \|\pi - \pi_h\|_{L^{p'}} = \mathcal{O}(h^{2/p'}),$$

provided that the solution has the natural regularity $\mathcal{F}(\mathcal{D}\mathrm{v}) \in W^{1,2}(\Omega)^{d\times d}$ and $\pi \in W^{1,p'}(\Omega)$. Here, the nonlinear function $\mathcal{F}(\cdot) : \mathbb{R}^{d\times d} \to \mathbb{R}^{d\times d}_{\mathrm{sym}}$ is defined by $\mathcal{F}(\mathcal{B}) = \big(\varepsilon + |\mathcal{B}_{\mathrm{sym}}|\big)^{(p-2)/2}\mathcal{B}_{\mathrm{sym}}$, For $p > 2$, the following estimates are proven:

$$\|\mathcal{F}(\mathcal{D}\mathrm{v}) - \mathcal{F}(\mathcal{D}\mathrm{v}_h)\|_{L^2} = \mathcal{O}(h^{p'/2}), \quad \|\mathrm{v} - \mathrm{v}_h\|_{W^{1,p}} = \mathcal{O}(h^{1/(p-1)}), \quad \|\pi - \pi_h\|_{L^{p'}} = \mathcal{O}(h^{p'/2}).$$

These results improve those in the literature with respect to order and regularity requirements. Their sharpness is confirmed by a series of carefully designed numerical tests. However, these tests also show that for $p > 2$ not all of these estimates seem to be order-optimal. This effect is likely due to nonoptimal estimation of certain error terms and, in the case of the pressure error, certainly due to super-approximation on uniform meshes. This question requires further investigation. The chapter is closed by an analysis of the full discretization of the nonstationary p-Stokes equations by the spatial discretization as described above combined with the (implicit) backward Euler time discretization. Using standard arguments from the literature several error estimates are derived, e.g., for $p \in (3/2, 2]$ and $d = 3$:

$$\max_{0\le n\le N} \|\mathrm{v}(t_n) - \mathrm{v}^n\|_{L^2} + \Big(k\sum_{n=0}^{N} \|\mathcal{F}(\mathcal{D}\mathrm{v}(t_n)) - \mathcal{F}(\mathcal{D}\mathrm{v}^n)\|_{L^2}^2\Big)^{1/2} = \mathcal{O}(h^{3p/4-1/2} + k).$$

However, for $p < 2$ the obtained orders of convergence are lower order than those known from the literature for standard parabolic problems with nonlinearity of p-structure. The difficulty is caused by the differential-algebraic character of the Stokes equations and lacking bounds for the discrete pressures. This question is carefully discussed and several ideas for its solution are given. However, the final answer is left as an open problem.

In Chapter 5 the results of the preceding chapter are extended to the full (nonstationary) p-Navier-Stokes equations. First, the standard LPS stabilization technique is used to stabilize the transport term in the p-Oseen equations, which occur as intermediate steps within the linearization and time discretization of the p-Navier-Stokes equations. Using the techniques from Chapter4 for the case $p \in (1,2]$ corresponding optimal-order a priori error estimates are derived for the present situation. These theoretical results are again confirmed by a series of numerical tests. In this context also the treatment of others than the usual "no-slip" boundary condition is discussed. For practical purposes the most important one is the so-called "do nothing" outflow boundary condition which models "free parallel" outflow as typically occurring in pipe flow. Then, the DWR approach for "goal-oriented" a posteriori error estimation and mesh optimization is developed for the p-Navier-Stokes equations. This follows similar developments for nonlinear problems in the literature. Several numerical tests including a standard channel flow benchmark confirm the effectivity of the DWR method for the p-Navier-Stokes equations.

Then, in Chapter 6 the finite element approximation of the "singular" power-law system

$$\mathcal{S}(|\mathcal{D}|^2) = \mu_0|\mathcal{D}|^{p-2}\mathcal{D}, \quad p \in (1,2),$$

is considered. In this model vanishing shear stress results in unbounded viscosity. Here, the spatial discretization is assumed to be by an "inf-sup"-stable finite element pair (e.g., Taylor-Hood Stokes element) in order to simplify the presentation. By mesh-dependent regularization of the form

$$\mathcal{S}_\varepsilon(|\mathcal{D}|^2) = \mu_0\big(\varepsilon(h)^2 + |\mathcal{D}|^2\big)^{(p-2)/2}\mathcal{D}, \quad p \in (1,2),$$

Newton convergence is achieved with controllable convergence rate. The corresponding error estimates

$$\|\mathrm{v} - \mathrm{v}_h^\varepsilon\|_{W^{1,p}} = \mathcal{O}(\varepsilon^{p/2} + h), \quad \|\pi - pi_h^\varepsilon\|_{L^{p'}} = \mathcal{O}(\varepsilon^{p-1} + h^{2/p'}),$$

are confirmed by numerical tests. The optimal choice is $\varepsilon(h) = h^{2/p}$.

Finally, in Chapter 7 the case of shear-rate and pressure dependent viscosity is considered. The well-posedness of the discretized systems is shown together with qualitative convergence without requiring any extra regularity. For $p \in (1,\infty)$ and $\varepsilon > 0$ again a priori error estimates are derived and confirmed by numerical tests. For these results the pressure dependence has to be assumed to be only sublinear with a sufficiently small coefficient. The treatment of general superlinear dependence, which would be more realistic for practical applications, seems out of reach yet with respect to theoretical analysis of the models as well as their numerical approximation.

The thesis closes with Conclusions and Outlook (Chapter 8) summarizing the main results obtained.

Evaluation: This thesis deals with a numerical problem of high complexity reflected by the many open questions posed at the beginning. It contains an overwhelmingly rich collection of single results. The analytical arguments are correct. Further, it is remarkable how systematically all theoretical claims on convergence properties have been investigated by numerical tests with positive confirmation in most cases. In this respect the thesis represents an enormous amount of work of high scientific quality and originality. However, many ideas and arguments have been taken from the literature though with significant improvements and extensions. But there is no really big "result" or "breakthrough", which opens the path for further research directions and deserves the rating "excellent".

I rate this doctoral thesis by very good (1,0)

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