Referee's Comments on the Doctoral Thesis

Towards efficient numerical computation of flows of non-Newtonian fluids
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This excellent doctoral thesis is concerned with the mathematical analysis and numerical approximation of mathematical models for non-Newtonian fluids.

The stable, accurate, reliable, and efficient numerical approximation to solutions of nonlinear partial differential equations is an active and important field of current research. Much of the research to date has concentrated on the development and mathematical analysis of numerical algorithms for viscous incompressible Newtonian fluids, while for non-Newtonian fluids the construction and analysis of numerical schemes have lagged behind.

Non-Newtonian fluids play a significant role in one's daily life, and their ubiquity is undeniable: they range from cosmetic and household products, such as creams, gels, paints, pastes, but are also of important use in industry (e.g. asphalt in road and motorway construction).

In this respect, the thesis addresses an important class of mathematical models, in the impressive research tradition of the Nečas Center for Mathematical Modelling over the past decade.

The thesis is structured as follows. In the first part of the thesis the candidate discusses the constitutive theory of incompressible fluids characterized by a continuous monotone relation between the velocity gradient and the Cauchy stress. In particular, he investigates a class of activated fluids, which behave like an Euler fluid prior to activation, and as a Navier–Stokes or power-law type fluid following the activation. He establishes the existence of large-data global weak solutions for both steady and unsteady three-dimensional flows of such fluids subject either to a no-slip boundary condition or to a range of slip-type boundary conditions, including free-slip, Navier's slip, and stick-slip boundary condition.

In the second part of the thesis the candidate focuses on an important question in a posteriori error analysis of finite element methods. The purpose of a posteriori error analysis is to derive a computable bound, in a suitable norm, for example, on the difference between the computed solution and the unknown analytical solution of a partial differential equation. A posteriori error bounds involve the finite element residual, obtained by substituting the computed numerical solution into the partial differential equation under consideration, in order to quantify the extent to which the numerical solution fails to satisfy the partial differential equation. Typically, such finite element residuals in a posteriori error bounds for second-order elliptic problems appear in terms of their negative Sobolev norm, $\|\cdot\|_{W^{-1,q}(\Omega)}$, simply because $W^{-1,q}(\Omega)$, for $q \in (1, \infty)$, is the natural function space for the data in weak formulations of (linear and nonlinear) second-order elliptic partial differential equations. The fact that the

$W^{-1,q}(\Omega)$-norm is nonlocal in nature has unpleasant consequences from the point of view of a posteriori error estimation, as one would, ideally, like to identify local subregions within the computational domain Ω where the current numerical approximation is inaccurate and improve its accuracy by local mesh-refinement. Therefore the results in the second part of the candidate's thesis are of marked importance. He shows that the negative Sobolev norm $W^{-1,q}(\Omega)$ is localizable, provided that the functional in question vanishes on locally supported functions which constitute a partition of unity. The main result of Chapter II is Theorem II.3.7. This result represents a key tool for establishing local a posteriori efficiency for partial differential equations in divergence form with residuals that belong to the Sobolev space $W^{-1,q}(\Omega)$. A simple generalization of the main result is provided in Theorem II.4.1, and in Example II.4.6 the candidate links the approach, in a simplified setting, to ℓ^2-estimates of the algebraic residual. He demonstrates that the approach of Theorem II.4.1 may be too crude to be efficient. Theorem II.4.3 together with Example II.4.4 gives a remedy for this problem; it requires a more complicated approach, but it allows one to recover local efficiency. Section II.5 presents a numerical example, which supports the theoretically obtained results.

In the third part of thesis the candidate provides a new analysis for a pressure convection-diffusion preconditioner. The development of efficient preconditioners is an important branch of Numerical Linear Algebra, as the performance of iterative solvers for large systems of linear algebraic equations that arise from the discretization of partial differential equations can be significantly improved by the use of efficient preconditioners. Surprisingly, the traditional approach in this area of Numerical Linear Algebra focussed on the construction of preconditioners in a manner that ignored the natural infinite-dimensional functional-analytic setting of the partial differential equations, from which the system of linear equations arose in the course of the numerical approximation. It has been recorgised in recent years (as evidenced for example by the work of Mardal & Winther, Numer. Linear Algebra Appl. 2011; 18:1–40, the work of R. Kirby, SIAM Rewview, 2010; 32:269–293, or the excellent 2015 SIAM book by Málek & Strakoš: Preconditioning and the conjugate gradient method in the context of solving PDEs) that it is a conceptual mistake to attempt to develop preconditioners in this way, by ignoring the infinite-dimensional problem from which the finite-dimensional problem arose. In this spirit, the candidate first develops a theory for the preconditioner considered as an operator in infinite-dimensional spaces. He then provides a methodology for constructing discrete pressure convection-diffusion operators for a wide class of pressure discretizations. The principal contribution of the candidate's work is that he provides an efficient methodology for dealing with artificial boundary conditions, including the case of inflow-outflow boundary condition, which have not been adequately addressed in the existing literature. Specifically, Section III.2.2 investigates conditions under which the pressure convection-diffusion operator is guaranteed to be well-defined and invertible on appropriate spaces, and provides uniform estimates for its norm and spectrum. A novel aspect of the candidate's approach is the relaxation of the requirements on the regularity and the divergence of the convective field. An important observation regarding the structure of the preconditioned Schur complement appears in (III.2.54): it asserts that the preconditioned Schur complement is a compact perturbation of the Stokes Schur complement, which is a positive self-adjoint operator. In Section III.2.4 the candidate shows that the perturbation is of $(6 + \epsilon)$-Schatten class, and that this implies that the spectrum of the preconditioned Schur complement accumulates at the spectrum of the Stokes Schur complement with the rate $6 + \epsilon$. In Section III.2.5 the candidate discusses the implications of this theoretical result for the convergence of the GMRES method. Section III.2.6 of the thesis discusses the relation of two pressure convection-diffusion variants and of the boundary conditions imposed in the definition of the pressure convection-diffusion operators. Section III.3.1 provides a methodology for the construction of discrete pressure convection-diffusion operators for a broad class of pressure discretizations, including the case of inflow-outflow boundary conditions. The main results of Chapter III are Theorems III.3.2 and III.3.3, which guarantee invertibility of and a priori bounds on discrete pressure convection-diffusion operators under appropriate conditions. The subsequent sections then derive particular forms of the pressure convection-diffusion operator for specific discretizations. In Section III.3.5 the candidate elaborates on some aspects of previously published accounts and compares these to his results.

The exposition in the thesis is clear and scholarly throughout. The work reported in the thesis represents a significant new scientific contribution to the numerical approximation of mathematical models of incompressible fluids, and clearly demonstrates the candidate's ability to undertake high-quality creative scientific work.

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