Lawrence Berkeley National Laboratory

Recent Work

Title

ON THE NUMERICAL INTEGRATION OF VISCOELASTIC FLOW EQUATIONS

Permalink

https://escholarship.org/uc/item/79c2g894

Authors

Rosenberg, J. Keunings, R.

Publication Date 1988-10-01

LBL-26467

BL-2646

Center for Advanced Materials				

MAR 3 1989

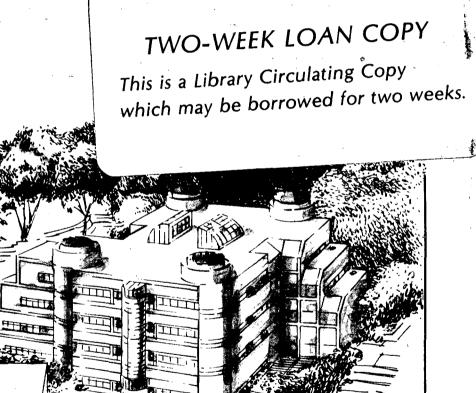
LIBRARY AND DOCUMENTS SECTION

To be presented at the Seventh International Conference on Finite Element Methods in Flow Problems, Huntsville, AL, April 3–7, 1989, and to be published in the Proceedings

On the Numerical Integration of Viscoelastic Flow Equations

J. Rosenberg and R. Keunings





Materials and Chemical Sciences Division Lawrence Berkeley Laboratory • University of California ONE CYCLOTRON ROAD, BERKELEY, CA 94720 • (415) 486-4755

Prepared for the U.S. Department of Energy under Contract DE-AC03-76SF00098

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

ON THE NUMERICAL INTEGRATION OF VISCOELASTIC FLOW EQUATIONS

by

J. Rosenberg and R. Keunings

October 1988

to be published in the Proceedings of the Seventh International Conference on Finite Element Methods in Flow Problems April 3-7, 1989, Hunstville, Alabama, USA

1

 \mathcal{T}

ON THE NUMERICAL INTEGRATION OF VISCOELASTIC FLOW EQUATIONS

J. Rosenberg and R. Keunings^{*} Center for Advanced Materials, Lawrence Berkeley Laboratory University of California, Berkeley CA 94720, USA

Abstract

Various numerical techniques are compared in the integration of the upper-convected Maxwell (UCM) constitutive model on the basis of known kinematics. They include Galerkin's method, streamline upwinding schemes and the method of characteristics. The results show the superiority of the latter in flows endowed with stress singularities. Solutions of the full set of momentum, mass and constitutive equations are computed with the method of characteristics and a Picard iterative scheme. Convergence difficulties are addressed.

1. Introduction

In the past, Galerkin finite element methods (GFEM's) have been the techniques of choice in the numerical discretization of viscoelastic flow equations (see [1] and [2] for detailed reviews). GFEM's, however, are known to produce oscillatory results in flow problems possessing stress singularities or boundary layers, with the consequence that solutions can only be obtained for small values of the Weissenberg number. (The Weissenberg number We is a dimensionless group determining the elastic character of the flow [1,2]). One cause for the numerical instabilities is related to the hyperbolic nature of differential viscoelastic constitutive models [1].

In the first part of the present communication, various methods are compared in the prediction of viscoelastic stresses on the basis of known kinematics for the planar stick-slip problem. The methods include Galerkin's technique, streamline upwinding (SU), streamline-upwind Petrov-Galerkin (SUPG), and streamline integration (SI) applied to the integration of the UCM constitutive model. In the second part, a Picard iterative method is used together with SI to produce solutions of the full set of governing equations for an Oldroyd-B fluid. Convergence behavior of the iterations is discussed. For a complete written report, see [3].

2. Governing Equations

Isothermal creeping flow of an Oldroyd-B fluid is governed by the following equations :

$\lambda T_{v}^{\nabla} + T_{v} = 2 \mu_{v} D ,$	(1)
$\nabla .(2 \mu_N D + T_v - p I) + f = 0$,	(2)
$\nabla . \mathbf{u} = 0$.	(3)

13

Here λ is a relaxation time, μ_v and μ_N are viscoelastic and Newtonian viscosity coefficients respectively, D is the rate of deformation tensor, u is the velocity vector, p is pressure, f is a body force, T_v is the viscoelastic extra-stress tensor, and the superscript ∇ refers to the upperconvected derivative [1]. By setting appropriate parameters to zero, these equations also

^{*} Permanent address : Unité de Mécanique Appliquée, Université Catholique de Louvain, Place du Levant 2, 1348 Louvain-la-Neuve, Belgium

describe Newtonian and Maxwell (UCM) flows. For fixed steady-state kinematics, the UCM equation (1) constitutes a set of first-order hyperbolic equations for T_{y} .

3. Numerical Techniques

The governing equations (1-3) are usually solved in terms of the primary variables T_v , u, and p by means of a GFEM [1]. The unknown fields are approximed by the finite sums :

$$T_{\mathbf{v}} = \sum_{i} T_{\mathbf{v}i} \phi_{i} , \quad \mathbf{u} = \sum_{j} u_{j} \psi_{j} , \quad \mathbf{p} = \sum_{k} p_{k} \pi_{k} , \quad (4)$$

where T_{vi} , u_j , and p_k are unknown nodal values, and ϕ_i , ψ_j , and π_k are finite element basis functions. For planar flows, the standard Galerkin weak form of (1-3) is

$$<\phi_{i}; \lambda T_{v} + T_{v} - 2\mu_{v} D > = 0,$$
 (5)

$$\langle \nabla \psi_{j}^{I}; 2 \mu_{N} D + T_{v} - p I \rangle = \langle \langle \psi_{j}; t \rangle + \langle \psi_{j}; f \rangle, \qquad (6)$$

 $<\pi_{\mathbf{k}}; \nabla .\mathbf{u} > = 0, \tag{7}$

where the brackets $\langle ; \rangle$ and $\langle \langle ; \rangle \rangle$ denote the L² inner products over the flow domain and the domain boundary respectively, and t is the surface traction. In this work, the elements used are isoparametric quadrilaterals, extra-stress and pressure approximations are bilinear, and velocity interpolations are biquadratic. All approximations are of class C⁰. Following [4], the extra-stress is calculated on a mesh where each quadrilateral is subdivided uniformly into NxN sub-elements, with N between 1 and 4.

3.1. Integration of the Constitutive Equation

GFEM's are known to be unstable in the solution of hyperbolic problems [5]. Various upwinding techniques have been introduced recently to stabilize finite element solutions of hyperbolic systems, most notably streamline upwinding (SU) and streamline-upwind Petrov-Galerkin (SUPG) methods (see e.g. [6]).

SU as applied to the constitutive model (1) essentially amounts to solving the modified equation

$$\nabla \cdot (K \nabla T_v) + \lambda T_v + T_v = 2 \mu_v D.$$
(8)

Here the tensor K, the anisotropic artificial diffusivity tensor, is given by

$$K = k \frac{u u}{u \cdot u}, \tag{9}$$

where k is a scalar on the order of element size.

SUPG solves the original constitutive equation (1) but uses a weight function differing from the basis function :

2

$$< w_i^{}\,;\,\lambda\stackrel{\nabla}{T}_{\!\nu} + T_{\!\nu}^{}$$
 - 2 $\mu_{\!\nu}^{}\,D> = 0$,

(10)

ß

where c is also a scalar on the order of element size.

In 2-D steady-state flows, the streamlines are the characteristic lines for the hyperbolic constitutive model (1). Streamline integration (SI) is a method by which the constitutive equations are integrated along the particle paths [7]. First, streamlines are computed on the basis of a known velocity field. A second order A-stable adaptive method is then used to numerically integrate (1) along a discrete number of streamlines. The integration stepsize along a particle path is adjusted such that an estimate of the relative discretization error does not exceed some predefined tolerance.

3.2. Solution of the Full Set of Equations

Following [7], SI is used within a decoupled method [1] to predict viscoelastic extrastress and kinematics for the Oldroyd-B fluid. The iterative method, henceforth referred to as SLE, is as follows :

- (1) Determine Newtonian kinematics via GFEM,
- (2) For each Gauss-point on a NxN sub-mesh, determine new values for T_v via SI on the basis of current kinematics,
- (3) Determine kinematics based upon T_v via the Galerkin equations

<
$$\nabla \psi_{j}^{T}$$
; 2($\mu_{a} + \mu_{N}$) $D^{N+1} - p^{N+1} I >$
= < $\nabla \psi_{j}^{T}$; 2 $\mu_{a} D^{N} - T_{v}^{N} > + << \psi_{j}$; t >> + < ψ_{j} ; f > , ⁽¹²⁾

 $<\pi_k$; $\nabla . u^{N+1} > = 0$,

where the superscripts denote the iteration index.

(4) Check for convergence. Return to step (2) if necessary.

An "arbitrary" viscosity μ_a is added to both sides of (12) to aid convergence of the iterative process. Following [7], the finite elements are made to conform with the streamlines computed at each iteration, so that families of Gauss-points lie on common paths.

Convergence of SLE is expected to be first order at best. Unlike for Newton-Raphson iterations, convergence criteria for SLE are not altogether obvious. *Maximum relative changes* (MRC's) are defined by

$$\frac{\max_{g} |T_{vg}^{N+1} - T_{vg}^{N}|}{\max_{g} |T_{vg}^{N+1}|}, \frac{\max_{j} |u_{j}^{N+1} - u_{j}^{N}|}{\max_{j} |u_{j}^{N+1}|},$$
(14)

where the subscript g refers to Gauss-points. Similar MRC's are also defined for pressure and streamfunction. *Residuals* are defined by

$$R = || < \nabla \psi_{j}^{T}; 2 \mu_{N} D^{N+1} - p^{N+1} I + T_{v}^{N+1} > - <<\psi_{j}; t >> - <\psi_{j}; t >||_{2}.$$
(15)

(13)

Finally, *distances* are defined by

$$\left\| T_{vg}^{N+1} - T_{vg}^{0} \right\|_{2}, \left\| u_{j}^{N+1} - u_{j}^{0} \right\|_{2},$$
 (16)

again where similar quantities are defined for pressure and streamfunction. The superscript 0 in (16) refers to a particular (fixed) iterate. *Convergence of the iterative process* is defined here as the situation when all MRC's remain below 0.05 and all residuals and distances do not diverge over prolonged iterations.

4. Results for Newtonian Kinematics

The planar stickslip problem [1] is chosen to test the various techniques of solving the differential constitutive equation (1). The Newtonian kinematics are determined via GFEM. GFEM, SU, SUPG, and SI are then used to predict the UCM extra-stress for We=3 on the basis of the computed Newtonian kinematics.

In the full report [3], the predictions of these various techniques are compared along several streamlines for 1x1, 2x2, and 4x4 sub-meshes for the extra-stress computation. In summary, Galerkin, SU, and SUPG are inaccurate in the exit region where a steep stress boundary layer is predicted in the direction transverse to the flow. Away from the exit region, SU and SUPG give accurate results when a 4x4 sub-mesh is used. SI results are the most stable and accurate; they do converge with increased resolution even near the exit.

5. Results with the Decoupled Method

Performance of SLE is tested on the stickslip flow problem of an Oldroyd-B fluid with viscosity ratio $\mu_N/\mu_v=1/8$. Iterations for a 1x1 sub-mesh begin at We=0 and continue until convergence is lost slightly above We=1/2. SLE with 4x4 sub-mesh refinement is used in a similar test. At We=1/2, convergence has already been lost (without catastrophic divergence) with the MRC in stresses being on the order of unity. The 4x4 sub-refinement requires evaluation of stress much closer to the singularity than does its 1x1 counterpart. An MRC in velocity on the order of 0.01 can produce an MRC in stress on the order of 1 in the elements close to the singularity.

In this work, the arbitrary viscosity μ_a is chosen by trial and error. If μ_a is too low, the iterations diverge wildly. If μ_a is chosen too high, the computed MRC's are deceptively low, but the solution nevertheless can diverge with prolonged iterations. Typically, convergence (when it does occur) is slow and oscillatory. SLE on the 1x1 sub-mesh takes on the order of 200 iterations at the total cost of about 8 CPU minutes on a CRAY X-MP (single processor) to obtain converged results for We=1/2.

6. Conclusions

Current boundary conditions and constitutive models used in viscoelastic flow modeling often result in physically unreasonable stress and stress gradients. In the predicted boundary layers, small changes in kinematics can produce large changes in the computed stress field. Finite element upwinding techniques for viscoelastic extra-stress calculation have been shown to be an improvement over standard Galerkin methods. They do not, however, produce accurate results close to singularities. The streamline integration of the UCM constitutive model leads to stable and accurate stress predictions even near the singularity. A decoupled technique based on streamline integration does not, however, enjoy good convergence properties and fail to converge at rather low values of We. This work also shows that convergence criteria for decoupled viscoelastic iterations must be carefully defined.

2

Acknowledgments

This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Materials Science Division of the US Department of Energy under Contract N° DE-AC03-76SF00098. The numerical simulations described in this paper have been conducted on a CRAY X-MP supercomputer of the National Magnetic Fusion Energy Computer Center, Lawrence Livermore National Laboratory.

References

- Keunings R., Simulation of Viscoelastic Fluid Flow, in <u>Fundamentals of Computer</u> <u>Modeling for Polymer Processing</u>, C.L. Tucker III, Editor, Carl Hanser Verlag, in press (1988)
- [2] Crochet M.J., Numerical Simulation of Viscoelastic Flow : a Review, Rubber Chemistry and Technology, Rubber Reviews, Amer. Chem. Soc., in press (1988)
- [3] Rosenberg J. and Keunings R., in preparation
- [4] Marchal J.M. and Crochet M.J., J. Non-Newt. Fluid Mech., <u>26</u>, 77 (1987)
- [5] Johnson C., Navert U. and Pitkaranta J., Comp. Meth. Appl. Mech. Engng., <u>45</u>, 285 (1984)
- [6] Brooks A.N. and Hughes T.J.R., Comp. Meth. Appl. Mech. Engng., <u>32</u>, 199 (1982)
- [7] Luo X.L. and Tanner R.I., J. Non-Newt. Fluid Mech., <u>21</u>, 179 (1986)

LAWRENCE BERKELEY LABORATORY CENTER FOR ADVANCED MATERIALS 1 CYCLOTRON ROAD BERKELEY, CALIFORNIA 94720