LA-UR- 96-2751

CONF-9610173--1

Title: THREE-DIMENSIONAL FINITE ELEMENT SIMULATION OF VISCOELASTIC FLUID FLOW USING THE EVSS-G

Author(s): A. Benard, P. M. Lovalenti, D. L. Tullock, E. D. Montalbano, D. C. Guell

Submitted to: IACHE Annual Conf., Chicago, IL, October 1996

Los Alamos
NATIONAL LABORATORY

Form No. 836 R5
ST 2629 10/91

DISCLAIMER

Three-dimensional finite element simulation of viscoelastic fluid flow using the EVSS-G

A. Benard, P.M. Lovalenti, D.L. Tullock, E.D. Montalbano and D.C. Guell
Los Alamos National Laboratory, Los Alamos, NM 87545

Abstract

An implementation of the EVSS-G method in a finite element framework is presented for modeling three-dimensional viscoelastic flows. The extension from two to three dimensions is discussed, along with the use of the Picard and Newton-Raphson iterative techniques. A selection of benchmark problems, with known analytical solutions are presented as validation of the implementation as well as results for secondary flows in rectangular ducts.

Injection molding simulation software typically uses the Hele-Shaw approximation to formulate the governing equations. However, as molded parts become increasingly complex and filling times become shorter, three-dimensional and viscoelastic effects that cannot be included in such a treatment may become important [1]. Recently, the EVSS-G method (elastic-viscous split stress) has been introduced for simulation of two-dimensional viscoelastic flows [2]. As computer power increases, extending such methods to three-dimensional flows becomes more feasible.

In this paper, after a brief review of the governing equations, implementation issues for the EVSS-G method are discussed. These issues involve the use of the Picard iterative method together with the Newton-Raphson iterative scheme. Results for problems such as flow in a duct with weak secondary vortices will also be presented.

GOVERNING EQUATIONS

The governing equations for steady, isothermal, viscoelastic flow are presented in this section. The equations include the continuity equation, given by

$$\nabla \cdot \mathbf{v} = 0, \tag{1}$$

for an incompressible fluid. The momentum equation is written in dimensional form as

$$\rho \mathbf{v} \cdot \nabla \mathbf{v} + \nabla \cdot \boldsymbol{\tau} + \nabla p = 0, \tag{2}$$

where ρ is the fluid density, $\mathbf{v}$ the velocity, and p the pressure. In viscoelastic constitutive equations, the deviatoric stress tensor $\boldsymbol{\tau}$ is often divided into a polymer contribution $\boldsymbol{\tau}_p$ and a solvent contribution $\boldsymbol{\tau}_s$, i.e.$\boldsymbol{\tau} = \boldsymbol{\tau}_p + \boldsymbol{\tau}_s$, and where $\boldsymbol{\tau}_s = -\eta_s \dot{\boldsymbol{\gamma}}$. $\dot{\boldsymbol{\gamma}}$ is the rate-of-strain tensor

and η_s is the solvent viscosity. In the EVSS/EVSS-G formulations, another change of variable is introduced, i.e. $\mathbf{\Sigma} \equiv \boldsymbol{\tau}_p + \eta_p \dot{\boldsymbol{\gamma}}$, where $\mathbf{\Sigma}$ corresponds to the elastic part of the deviatoric stress [3]. Combining these variable changes provides $\boldsymbol{\tau} = \mathbf{\Sigma} - \eta_o \dot{\boldsymbol{\gamma}}$, and substituting into the momentum equation yields

$$\rho \ \mathbf{v} \cdot \boldsymbol{\nabla}\mathbf{v} + \boldsymbol{\nabla} \cdot \mathbf{\Sigma} - \eta_o \boldsymbol{\nabla}^2 \mathbf{v} + \boldsymbol{\nabla} p = 0. \tag{3}$$

This change of variables has the advantage of yielding the viscous operator $\boldsymbol{\nabla}^2\mathbf{v}$ unweighted by the solvent viscosity so that problems in which $\eta_s = 0$ can be solved. Also, the mathematical type of the equation set is strictly elliptic for velocity and pressure and strictly hyperbolic for stress [3]. In the EVSS-G method, the velocity gradients are treated as additional unknowns in the problem and approximated by Lagrange linear basis functions. The additional equations required are provided by the definition of the velocity gradient, i.e. $\mathbf{G} \equiv \boldsymbol{\nabla}\mathbf{v}$.

For the Giesekus model, the polymer contribution to the stress satisfies

$$\boldsymbol{\tau}_p + \lambda_1 \boldsymbol{\tau}_{p(1)} - \alpha \frac{\lambda_1}{\eta_p} (\boldsymbol{\tau}_p \cdot \boldsymbol{\tau}_p) + \eta_p \dot{\boldsymbol{\gamma}} = 0. \tag{4}$$

which can be used with the Newton-Raphson method discussed below. For the Picard iterative method, another more complex form of this equation is required, with $\mathbf{\Sigma}$ as dependent variable. This form is obtained when the change of variables $\mathbf{\Sigma} \equiv \boldsymbol{\tau}_p + \eta_p \dot{\boldsymbol{\gamma}}$ is introduced.

The equations were discretized using the standard Galerkin formulation but are omitted here for the sake of brevity. The weight and shape functions employed were all linear, except for the velocities, which were quadratic. In addition, the streamline-upwind-Petrov-Galerkin method was applied to the constitutive equation. The features of this technique are discussed in several papers for two dimensional problems and the reader is encouraged to refer to them for further information [2,3].

IMPLEMENTATION ISSUES

A frontal solution technique was employed to solve the discretized system of linear equations [4]. Picard and Newton Raphson iterative methods are used to solve the non-linear system of equations. Typically, two or three Picard iterations were used first to bring the solution within the radius of convergence of the Newton-Raphson scheme, which is then used to bring the solution to the required degree of convergence.

For the Picard iterative method, the implementation of the equations is straightforward, but is also rather tedious due to the complexity of the constitutive equation that emerges after the change of variables. With Picard's Method, the full matrix for the equations based on $\mathbf{\Sigma}$, $\dot{\boldsymbol{\gamma}}$,$\mathbf{v}$ and P must be used as it requires that the following system be solved

$$\bar{\mathbf{K}}(\mathbf{U}^n)\mathbf{U}^{n+1} = \bar{\mathbf{F}}(\mathbf{U}^n), \tag{5}$$

where $\bar{\mathbf{K}}$ is the element matrix, $\mathbf{U}$ is the solution vector, and $\mathbf{F}$ is a forcing vector.

As mentioned above, Newton's method with analytical Jacobians was also employed. This method is actually somewhat more simple to implement due to simplifications that can be made in implementing Newton's Method and the EVSS-G together. In summary, Newton's method consists of solving

$$\mathbf{J}(\mathbf{U}^n)\Delta\mathbf{U} = -\mathbf{R}(\mathbf{U}^n) \tag{6}$$

for ΔU at each iteration and updating the variables U. J is the Jacobian matrix (or tangent matrix) given by

$$\mathbf{J} = \left.\frac{\partial \mathbf{R}}{\partial \mathbf{U}}\right|_{\mathbf{U}^n}, \tag{7}$$

and $\mathbf{R}$ is a vector containing the residuals of the equations. With this method, the entire set of equations need not be recast with $\boldsymbol{\Sigma}$ as the dependent variable. Instead, $\boldsymbol{\tau}_p$ can be used, which leaves the constitutive equation in its more simple form. Implementation of the combined EVSS-G/ Newton methods then consists of [5]

- Computing $\boldsymbol{\tau}_p$ from the previous iterate with $\boldsymbol{\tau}_p = \boldsymbol{\Sigma} - \eta_p \dot{\boldsymbol{\gamma}}$;
- Writing the residuals for the equations based on $\boldsymbol{\Sigma}$ ($\mathbf{R}(\boldsymbol{\Sigma})$) since they are identical to those based on $\boldsymbol{\tau}_p$ ($\mathbf{R}(\boldsymbol{\tau}_p)$), within numerical error;
- Computing the entries of the Jacobian matrix and employing the chain rule to compute the derivatives with respect to the velocity gradients.

Entries of the Jacobian matrix are then computed for the $\boldsymbol{\Sigma}$ formulation from the equations written with $\boldsymbol{\tau}_p$ as the dependent variable. The momentum equation is written in terms of $\boldsymbol{\Sigma}$ and the constitutive equation in terms of $\boldsymbol{\tau}_p$. Otherwise, the case $\eta_s = 0$ in the momentum equation results in a singular system of equations for $\mathbf{J}$. Also, when using Newton's method, the EVSS transformation, $\boldsymbol{\Sigma} \equiv \boldsymbol{\tau}_p + \eta_p \dot{\boldsymbol{\gamma}}$, takes place when the derivatives with respect to $\mathbf{G}$ are performed and the chain rule is used in computing the Jacobian matrix.

RESULTS

Our implementation of the method was tested satisfactorily against several known analytical solutions. These include simple shear and elongational flows, and a point source/sink problem based on a solution of Gartling [6]. Several interesting cases can be studied in three-dimensions. A popular one involves capturing the secondary vortices created by the flow of a viscoelastic fluid in a duct [7], which will be presented. The method was tested extensively and can be shown to require less memory than its predecessor the EVSS, from which it emerged. The method also proved to converge to higher De number than the EVSS for the source/sink flow problem.

LITERATURE CITED

1. D.C. Guell and P.M. Lovalenti, SPE 53rd Annual Conference, **1**, 728 (1995).
2. M.J. Szady, T.R. Salamon, A.W. Liu, D.E. Bornside, R.C. Armstrong, and R.A. Brown, J. Non-Newtonian Fluid Mech., **59**, 215 (1995).
3. D. Rajagopalan, R.C. Armstrong, and R.A. Brown, J. Non-Newtonian Fluid Mech., **36**, 159 (1990).
4. P. Hood, Int. J. Num. Meth. Eng., **10**, 379 (1976).
5. D. Rajagopalan, Personal Communication, 1996.
6. D.K. Gartling, J. Non-Newtonian Fluid Mech., **17**, 203 (1985).
7. S.C. Xue, N. Phan-Thien, R.I. Tanner, J. Non-Newtonian Fluid Mech., **59**, 191 (1995).