J. Non-Newtonian Fluid Mech. 151 (2008) 59–68

Journal of Non-Newtonian Fluid Mechanics

www.elsevier.com/locate/jnnfm

A timestepper approach for the systematic bifurcation and stability analysis of polymer extrusion dynamics

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Received 2 July 2007; received in revised form 13 September 2007; accepted 6 November 2007

Abstract

We discuss how matrix-free/timestepper algorithms can efficiently be used with dynamic non-Newtonian fluid mechanics simulators in performing systematic stability/bifurcation analysis. The timestepper approach to bifurcation analysis of large-scale systems is applied to the plane Poiseuille flow of an Oldroyd-B fluid with non-monotonic slip at the wall, in order to further investigate a mechanism of extrusion instability based on the combination of viscoelasticity and non-monotonic slip. Due to the non-monotonicity of the slip equation the resulting steady-state flow curve is non-monotonic and unstable steady states appear in the negative-slope regime. It has been known that self-sustained oscillations of the pressure gradient are obtained when an unstable steady state is perturbed [M.M. Fyrillas, G.C. Georgiou, D. Vlassopoulos, S.G. Hatzikiriakos, A mechanism for extrusion instabilities in polymer melts, Polymer Eng. Sci. 39 (1999) 2498–2504].

Treating the simulator of a distributed parameter model describing the dynamics of the above flow as an input–output "black-box" timestepper of the state variables, stable and unstable branches of both equilibrium and periodic oscillating solutions are computed and their stability is examined. It is shown for the first time how equilibrium solutions lose stability to oscillating ones through a subcritical Hopf bifurcation point which generates a branch of unstable limit cycles and how the stable periodic solutions lose their stability through a critical point which marks the onset of the unstable limit cycles. This implicates the coexistence of stable equilibria with stable and unstable periodic solutions in a narrow range of volumetric flow rates.

Keywords: Extrusion instabilities; Poiseuille flow; Oldroyd-B fluid; Bifurcation analysis; Timestepper approach; Floquet multipliers

1. Introduction

The complex viscoelastic character of polymers, the normal stress differences and the high extensional viscosity and wall slip may lead to non-linear phenomena and undesirable instabilities in polymer processing. Time-periodic phenomena are often observed, such as pressure oscillations at fixed volumetric flow rate in the stick-slip extrusion instability and draw resonance, which gives rise to spontaneous thickness and width oscillations in film casting, to a periodic fluctuation of the cross-sectional area in fiber spinning, and to periodic fluctuations of the bubble diameter in film blowing [1]. For example, draw resonance in the latter process corresponds to a self-sustained limit cycle type supercritical Hopf bifurcation [2]. In such flows, in addition to the steady-state solutions and linear stability, transient studies and non-linear stability analyses are necessary, in order to develop techniques for process optimization [2].

Modelling and understanding the mechanisms of such flow instabilities by determining the regions and the critical points where these occur are of major importance. For this purpose, the efficient simulation of the transient behavior of the underlying physical system, usually expressed in terms of a system of ordinary differential and algebraic equations or integro-partial differential algebraic equations, is required. Over the last years, some excellent temporal (direct integration in time) commercial

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0377-0257/$ – see front matter
doi:10.1016/j.jnnfm.2007.11.002

and home-made fluid mechanics simulation packages are the tools of choice. Such packages, which incorporate many man-years of effort and expertise, may also allow the computation of steady states using Newton-like solvers and comprise a very good option even for large-scale systems.

However, other important tasks, such as the exact location of the critical points that mark the onset of instabilities, as well as the dependence of the location on parameter values, cannot be obtained easily using temporal simulations. Furthermore, the tracing of branches of unstable steady states is often (in the absence of good initial guesses) impossible for large-scale systems. For the systematic and accurate analysis of the model dynamics, one has to resort to bifurcation analysis. Numerical bifurcation theory provides an arsenal of algorithms and software packages, such as AUTO, CONTENT and MATCONT for tasks such as the continuation of stable or unstable steady states and limit cycles, and the continuation of critical points [3–11]. While, these software packages are invaluable tools for performing systematic analysis for small- to medium-scale systems, there are some drawbacks in using them. Most of them require as input the system evolution equations, which are assumed to be explicitly available in discretized form. Linking the evolution equations with such packages is not a trivial task. These packages often use a Newton-like method, which requires the calculation of the Jacobian of the system (i.e. the matrix with the partial derivatives of the "right-hand-sides" of the discretized governing ODEs or the PDEs, with respect to the discrete unknowns). This imposes a serious computational burden in the analysis of large-scale systems. But even for small- to medium-size systems, tasks, such as the continuation of limit cycles or the continuation of turning points of limit cycles, become overwhelmingly computationally expensive or even prohibitive; these computations are usually performed by augmenting the system space with one more variable corresponding to the normalized time variable. The latter turns an initial-value problem to a boundary-value one, with a consequent vast increase in the size of the problem.

The solution to the "curse of dimensionality" comes from the matrix-free algorithms of iterative linear algebra [12] such as the Recursive Projection Method (RPM) of Shroff and Keller [13]. Here one does not need to numerically compute a matrix, such as the Jacobian of the system, in order to perform tasks such as solving, using for example the Newton method, systems of non-linear equations and stability analysis. What is required is the calculation of matrix-vector products which can be obtained by treating the dynamic simulators – the time integration codes (timesteppers) – as input–output "black-boxes" that take an initial condition and give the result of the integration after a prescribed time interval. These algorithms acquire the necessary information by calling the "black-box" timesteppers from appropriate nearby initial conditions and for relatively short-time intervals. This "wrapping" of matrix-free algorithms around industrial process simulators (like gPROMS) has been recently discussed by Siettos et al. [14] who applied the RPM for the efficient location of the cycle steady states and stability analysis of a periodically forced process.

The purpose of this paper is twofold: (a) to introduce the concept of matrix-free/timestepper approach that enables non-Newtonian fluid dynamics simulators to perform efficiently numerical stability/bifurcation analysis (such as continuation of both steady states and limit cycles and the computation of their stability); (b) to demonstrate the applicability of the method to viscoelastic flow problems in performing systematic numerical bifurcation and stability analysis of periodic solutions.

For the latter objective, the time-dependent, one-dimensional plane Poiseuille flow of an Oldroyd-B fluid with non-monotonic slip at the wall has been chosen. This problem has been considered by Georgiou and co-workers [15–17] who studied the combined effect of elasticity and non-monotonic slip and examined whether this can provide an explanation for the stick-slip extrusion instability [1]. All theoretical explanations suggested in the literature for this instability are based on the non-monotonicity of the flow curve (the plot of the wall shear stress versus the apparent shear rate, or, equivalently, the plot of the pressure gradient versus the volumetric flow rate), which exhibits a maximum and a minimum, and the fact that steady-state solutions corresponding to the negative-slope regime of the flow curve are unstable [18]. The transitions from the maximum of the flow curve to the right positive-slope branch and from the minimum to the left positive-slope branch lead to a limit cycle, which describes the observed pressure and flow rate oscillations in flow rate-controlled experiments [19].

Non-monotonicity of the flow curve can be obtained by a non-monotonic slip law (adhesive failure) or by a non-monotone constitutive equation (bulk failure). In the proposed explanations involving slip, this is combined with either compressibility or elasticity. The important role of slip in the stick-slip instability, indicated by both indirect and direct wall slip measurements, is also supported by the fact that only mechanisms involving slip lead to self-sustained pressure oscillations and generate waves on the extrudate surface. However, in addition to the experimental evidence for the importance of the compressibility of the melt in the reservoir, only the compressibility/slip mechanism can lead to persistent pressure and flow rate oscillations between the two stable branches of the flow curve. The periodic transitions between a weak slip (or no-slip) and a strong slip at the capillary wall (i.e. the jumps between the two branches of the flow curve) which lead to the pressure and flow rate oscillations are sustained by the compressibility of the melt in the reservoir. This mechanism has been employed in various one-dimensional phenomenological models describing the stick-slip instability (see [20] and references therein) and in two-dimensional simulations of both Poiseuille and extrudate-swell flows (see [19] and references therein).

Viscoelasticity may replace compressibility and, when combined with non-monotonic slip, can act as a storage of elastic energy generating self-sustained pressure oscillations and waves on the extrudate surface in the stick-slip regime. Due to the absence of compressibility, however, this mechanism cannot generate jumps of the volumetric flow rate between the two stable branches of the flow curve and leads only to small-amplitude small-wavelength distortions of the extrudate surface consistent with sharkskin rather than with the stick-slip instability.