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Application of full flow field reconstruction to a viscoelastic liquid in a 2D cross-slot channel

Monirosadat Sadati [a,*], Clarisse Luap [a], Beat Lüthi [b], Martin Kröger [a], Hans Christian Öttinger [a]

[a] Department of Materials, Polymer Physics, ETH Zürich, Wolfgang-Pauli-Str. 10, CH-8093 Zürich, Switzerland
[b] Institute of Environmental Engineering, ETH Zürich, Wolfgang-Pauli-Str. 15, CH-8093 Zürich, Switzerland

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ABSTRACT

High quality flow kinematics reconstruction from noisy and spatially scattered data requires the use of a regularization technique. Enforcing incompressibility, we employ the recently proposed Tikhonov regularization method combined with a high-order finite element approximation in its stream function formulation. The method is applied to experimental particle tracking velocimetry data, obtained for an incompressible polymer melt in a cross-slot channel. To overcome a potential regularization bias, where the velocity changes rapidly over small distances, regularization is performed on the departure of the velocity field from its Newtonian counterpart. It is compared with a more trivial approach, in which the data are smoothed locally and the velocity gradient fields computed using finite differences. The reconstructions are evaluated in terms of the quality of the streamlines and the velocity gradient histories. Regularization leads to significant noise reduction and to an improved utility of existing data for subsequent applications as we demonstrate by analyzing the principal stress-difference obtained by applying a constitutive equation to the reconstructed flow fields.

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1. Introduction

Recent experimental and numerical investigations have revealed that the dynamics of polymer chains in a mixed flow situation, in particular near a stagnation point, is far more complex than the dynamics of molecules in simple homogeneous shear and uniaxial stretching [1–9]. Within a viscoelastic polymeric liquid, the chains are imposed to different strain histories at different distances from the stagnation point. A better understanding to assess the performance of concentrated polymer solutions and melts in complex flows, where a mixture of shear and elongational deformation exists, can be fulfilled by accurately quantifying the flow kinematics to subsequently characterize shear and elongational properties of the fluid. With the flow kinematics at hand one can assess the performance of constitutive equations in predicting the stress field in mixed flows. A local fluid velocity is typically measured using particle tracking velocimetry or laser Doppler velocimetry. The accuracy of the constructed velocity field is an essential prerequisite for a reliable characterization of the kinematics and even more so for the reliability of the time-dependent information carrying the deformation history. The corresponding procedure is unfortunately far from being straightforward, for two reasons. First, the experimental complex flow data are usually acquired from a limited number of locations in the domain and contain undesired noise which can significantly alter the physical interpretation [8,9]. Second, evaluating constitutive equations to obtain the stress field from the experimental velocity data involves gradients of the velocity field. Therefore, reconstructing an accurate and complete velocity field from sparse and noisy data remains an important task. The reconstruction of a global velocity field and its gradients from noisy-scattered experimental data is an ill-posed problem because the solution is very sensitive to the presence of noise in the data. The solution of such a problem thus requires regularization. The Tikhonov regularization combined with high order finite element (FE) approximation had been proposed recently [10,11] as a robust technique for the reconstruction of full field flow kinematics from experimental velocity data. The main innovation of this method compared to others is its ability to reconstruct the variable and its derivative continuously over the whole field of interest where only a few randomly distributed values are available. The method was implemented and validated against synthetic noisy scattered data for an Oldroyd-B model fluid in a two dimensional (2D) complex flow situation. Within this approach the fluid incompressibility can be taken into account by either adding an extra term to penalize departures from incompressibility in the regularization procedure or by imposing it directly through a stream function formulation. We found that implementing the stream function approach is more effective in recovering the velocity information in a 2D incompressible flow

* Corresponding author. Present address: Program in Molecular and Integrative Physiological Sciences, School of Public Health, Harvard University, Boston, MA 02115, USA. Tel.: +1 857 756 0747.
E-mail address: sadati@hsph.harvard.edu (M. Sadati).

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situation [11]. It was elucidated that the best performance is achieved for an interpolation method using third order continuous Hermite FE shape functions, C^3, regularized by minimization of a norm of the velocity's third derivative.

We have performed the necessary experiment on a commercial viscoelastic liquid, a low density polyethylene melt, in an effectively 2D channel flow. With the data at hand we are going to critically investigate the performance of the proposed algorithm when for the first time applied to real experimental data. Section 2 describes the implementation of the Tikhonov regularization based on the stream function approach and the third order continuous Hermite FE approximation. Materials, methods and data acquisition is described in Section 3. The regularization method is applied in Section 4 on experimentally measured particle tracking velocimetry data in a cross-slot channel. The regularization quality is elucidated by using the regularized experimental flow kinematics to calculate the predicted stress field using the eXtended Pom-Pom (XPP) constitutive equation, which are then compared to the experimentally measured stress field. Concluding remarks will be offered in Section 5.

2. Tikhonov regularization

To obtain a continuous representation of a velocity field in 2D which preserves incompressibility, the reconstructed field (u^c, v^c) at any position $\mathbf{r}$ is expressed using the stream function-based finite element approximation [11]:

$$u^c(\mathbf{r}) = [\mathbf{N}_{,y}(\mathbf{r})]\mathbf{q}, \quad v^c(\mathbf{r}) = -[\mathbf{N}_{,x}(\mathbf{r})]\mathbf{q}, \tag{1}$$

where $[\mathbf{N}_{y}]$ and $[\mathbf{N}_{x}]$ are raw matrices containing the x, respectively y derivative of the third order continuous Hermite FE shape functions C^3 [11] of the element containing $\mathbf{r}$. The quantity $\mathbf{q}$ denotes the column vector formed by the stream function nodal values. From the experimentally measured velocity vector data, the unknown nodal values $\mathbf{q}$ are obtained by minimizing a cost functional. This functional χ is formed by a weighted least squares term minimizing the departure of the reconstructed field from the data, plus a regularization term penalizing the roughness of the velocity gradient,

$$\chi(\lambda) = \sum_{i=1}^{N} \frac{1}{(\sigma_i^u)^2}\left(u_i^c - \hat{u}_i^\sigma\right)^2 + \sum_{i=1}^{N} \frac{1}{(\sigma_i^v)^2}\left(v_i^c - \hat{v}_i^\sigma\right)^2 + \lambda \int_\Omega (\|f^{(3)}u^c(\mathbf{r})\|^2 + \|f^{(3)}v^c(\mathbf{r})\|^2) d^2r. \tag{2}$$

Here $u_i^c = u^c(\mathbf{r}_i)$ and $v_i^c = v^c(\mathbf{r}_i)$ denote the calculated values and $\hat{u}_i^\sigma$ and $\hat{v}_i^\sigma$ are experimentally measured values of the velocity field at N positions $\mathbf{r}_i$. The superscript σ indicates that the measured values, $\hat{u}_i^\sigma$ and $\hat{v}_i^\sigma$ come with standard errors of size σ_i^u and σ_i^v, respectively. The prefactor λ in Eq. (2) is the regularization parameter and sets the relative importance of smoothness versus interpolation. The norm $\|\cdot\|^2$ denotes the sum over all squared components; $f^{(3)}$ is a tensor of rank 3 containing all third derivatives, and the integrand of the regularization term, $\|f^{(3)}u^c(\mathbf{r})\|^2$ and likewise $\|f^{(3)}v^c(\mathbf{r})\|^2$ read

$$\|f^{(3)}u^c(\mathbf{r})\|^2 = \left(\frac{\partial^3 u}{\partial x^3}\right)^2 + 3\left(\frac{\partial^3 u}{\partial x^2 \partial y}\right)^2 + 3\left(\frac{\partial^3 u}{\partial x \partial y^2}\right)^2 + \left(\frac{\partial^3 u}{\partial y^3}\right)^2. \tag{3}$$

Substituting the finite element form of $u^c(\mathbf{r})$ and $v^c(\mathbf{r})$ given by Eqs. (1) and (3) into Eq. (2), the vector of nodal values $\mathbf{q}$ is calculated by minimizing Eq. (2), at a given regularization parameter, with respect to $\mathbf{q}$. From this vector, the complete velocity field components can be reconstructed at any position (Eq. (1)).

Application to scattered synthetic velocity data of an incompressible Oldroyd-B fluid with added random noise has shown that this method results in an efficient removal of the noise and an overall faithful reconstruction of the velocity field and velocity gradients [10,11]. However, the use of a single regularization parameter optimized over the whole domain leads to a small but systematic oversmoothing [11] at the corners of the channel, where a steep variation of the velocity gradient occurs.

To potentially limit this effect, we here apply the regularization procedure not directly to the velocity vector $(u(\mathbf{r}), v(\mathbf{r}))$ but to its departure $(\Delta u(\mathbf{r}), \Delta v(\mathbf{r}))$ from the velocity field expected for the corresponding incompressible Newtonian fluid,

$$\Delta u(\mathbf{r}) = u(\mathbf{r}) - u^{\text{newt}}(\mathbf{r}), \quad \Delta v(\mathbf{r}) = v(\mathbf{r}) - v^{\text{newt}}(\mathbf{r}). \tag{4}$$

The Newtonian velocity field $(u^{\text{newt}}(\mathbf{r}), v^{\text{newt}}(\mathbf{r}))$ can be generated for the given cross-slot geometry and input flow rate using any commercial finite element software and consequently be expressed in the chosen stream function based finite element approximation as

$$u^{\text{newt}}(\mathbf{r}) = [\mathbf{N}_{,y}(\mathbf{r})]\mathbf{q}^{\text{newt}}, \quad v^{\text{newt}}(\mathbf{r}) = -[\mathbf{N}_{,x}(\mathbf{r})]\mathbf{q}^{\text{newt}}. \tag{5}$$

Here $\mathbf{q}^{\text{newt}}$ regroups the nodal values for the corresponding Newtonian flow. Consequently, the unknown regularized departure from the Newtonian field is then given as:

$$\Delta u^c(\mathbf{r}) = [\mathbf{N}_{,y}(\mathbf{r})]\Delta\mathbf{q}, \quad \Delta v^c(\mathbf{r}) = -[\mathbf{N}_{,x}(\mathbf{r})]\Delta\mathbf{q}, \tag{6}$$

where $\Delta\mathbf{q} = \mathbf{q} - \mathbf{q}^{\text{newt}}$ is the difference in the stream function nodal value vectors for the calculated and Newtonian flow fields. As previously, the unknown $\Delta\mathbf{q} = \mathbf{q} - \mathbf{q}^{\text{newt}}$ is obtained by minimizing

$$\chi(\lambda) = \sum_{i=1}^{N} \frac{1}{(\sigma_i^u)^2}\left(\Delta u_i^c - \Delta\hat{u}_i^\sigma\right)^2 + \sum_{i=1}^{N} \frac{1}{(\sigma_i^v)^2}\left(\Delta v_i^c - \Delta\hat{v}_i^\sigma\right)^2 + \lambda \int_\Omega \left(\|f^{(3)}\Delta u^c(\mathbf{r})\|^2 + \|f^{(3)}\Delta v^c(\mathbf{r})\|^2\right) d^2r. \tag{7}$$

Defining the vector $\Delta\mathbf{b} = (\Delta\mathbf{b}^{uT} \quad \Delta\mathbf{b}^{vT})^T$ with $\Delta b_i^u = \Delta\hat{u}_i^\sigma/\sigma_i^u = (\hat{u}_i^\sigma - [\mathbf{N}_{,y}(\mathbf{r}_i)]\mathbf{q}^{\text{newt}})/\sigma_i^u$ and $\Delta b_i^v = \Delta\hat{v}_i^\sigma/\sigma_i^v$, the assembled matrix $\mathbf{K} = (\mathbf{K}^{uT} \quad \mathbf{K}^{vT})^T$ with $K_{ij}^u = N_{j,y}(\mathbf{r}_i)/\sigma_i^u$ and $K_{ij}^v = -N_{j,x}(\mathbf{r}_i)/\sigma_i^v$ and rewriting the regularization term as $\int_\Omega [\|f^{(3)}\Delta u^c(\mathbf{r})\|^2 + \|f^{(3)}\Delta v^c(\mathbf{r})\|^2] d^2r = \Delta\mathbf{q}^T\mathbf{R}_4\Delta\mathbf{q}$, Eq. (7) can be expressed in the following simple matrix form:

$$\chi(\lambda) = \|\mathbf{K}\Delta\mathbf{q} - \Delta \mathrm{b}\|^2 + \lambda\Delta\mathbf{q}^T\mathbf{R}_4\Delta\mathbf{q}, \tag{8}$$

where $\mathbf{R}_4$, the global regularization matrix of order $n = 4$, has been defined in [11]. The solution, at a given regularization parameter λ is obtained by minimizing Eq. (8) with respect to $\Delta\mathbf{q}$, which leads to [12]

$$\Delta\mathbf{q}^\lambda = (\mathbf{K}^T\mathbf{K} + \lambda\mathbf{R}_4)^{-1}\mathbf{K}^T\Delta \mathrm{b}. \tag{9}$$

As soon as the difference in the stream function nodal values $\Delta\mathbf{q}^\lambda$ is known, the velocity field can be reconstructed at any position $\mathbf{r}$ within the domain using

$$\mathbf{u}^{\text{rec},\lambda} = \mathbf{N}_{\text{rec},y}(\Delta\mathbf{q}^\lambda + \mathbf{q}^{\text{newt}}), \quad \mathbf{v}^{\text{rec},\lambda} = -\mathbf{N}_{\text{rec},x}(\Delta\mathbf{q}^\lambda + \mathbf{q}^{\text{newt}}), \tag{10}$$

where $\mathbf{u}^{\text{rec},\lambda}$ and $\mathbf{v}^{\text{rec},\lambda}$ are the vectors of reconstructed velocity values at a given regularization parameter λ and $\mathbf{N}_{\text{rec},y}$ and $\mathbf{N}_{\text{rec},x}$ stand for the assembled matrices of the first derivatives of shape functions corresponding to all wished new positions.

Therefore, by using this method with or without Newtonian subtraction, not only a smooth velocity field can be reconstructed but also calculation of the smooth gradient field is directly permissible. To achieve, for example the $\partial u/\partial x$ gradient field component in the reconstructing space, it is enough to replace $\mathbf{N}_{\text{rec},y}$ in Eq. (10) by the matrix of the corresponding cross derivative of shape functions, $\mathbf{N}_{\text{rec},yx}$.

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