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Numerical modelling of dispersive polymer blends

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Introduction
A well-known method for obtaining polymer materials with specific properties is blending multiple existing polymers. In this project, the evolution of the droplet morphology of immiscible dispersive polymer blends (See Figure 1) is studied using TFEM, an in-house developed FEM code.

Constitutive model
Based on [2], the morphology is described with monodisperse macroscopic droplet populations using the following morphology field variables: the deformation gradient tensor \( F \), the stretch ratio \( \beta \) and the unstretched droplet radius \( R_0 \). These variables are described using convection-type equations, which evolve over a Stokes velocity field:

\[
\nabla \cdot \mathbf{u} = 0, \quad -\nabla p + \nabla \cdot (2\mu_\text{e} \mathbf{D}) = 0, \\
\frac{\partial f}{\partial t} + \mathbf{u} \cdot \nabla f = g,
\]

where \( \mu_\text{e} \) is the effective blend dynamic viscosity (currently assumed constant), \( f \) is (a component of) a morphology variable and \( g \) is a nonlinear function that depends on the flow and morphological state.

Numerical simulation
In the example below (See Figure 2), the morphology development of a 10% PIB-90% PDMS mixture has been simulated in a channel with a cylindrical obstacle.

Results
The simulation was run until \( t = 30 \) with initially uniform \( \beta = 1 \) and \( R_0 = 10^{-2} \). Three illustrative frames have been plotted (See Figures 3 and 4):

Future work
The model yields qualitatively good results but needs to be experimentally validated. Points for future work are: (i) extending the model with polydisperse droplet populations, (ii) following the morphology evolution along a 3D particle path in complex flows and (iii) extending the model with viscoelasticity of the blend constituents.

References