Polymer chain simulations in microchannels with Dissipative Particle Dynamics
VASILEIOS SYMEONIDIS, MIT / Brown University, GEORGE KARNIADAKIS, Brown University, BRUCE CASWELL, Brown University — In this work we employ Dissipative Particle Dynamics (DPD) for simulations of dilute polymer solutions using bead-spring representations. We present comparison of two time-marching schemes: the popular velocity-Verlet and Lowe’s scheme. Schmidt number effects are investigated for a series of cases, including λ-DNA molecules under shear (using the Marko-Siggia wormlike chain spring law) and Poiseuille flow in microchannels. Effects on the polymer depletion layer, power-law profiles and apparent viscosities are presented as a function of the number of beads per polymer chain.