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Variable Cell Shape Methods in Polymer Field Theory Simulations GLENN FREDRICKSON, University of California, Santa Barbara, JEAN-LOUIS BARRAT, Universite Claude Bernard Lyon I and CNRS, SCOTT SIDES, University of California, Santa Barbara — We present a new method for carrying out field-theoretic simulations of inhomogeneous polymeric fluids under conditions of prescribed external stress, allowing for shape changes of the simulation cell. A compact expression for the deviatoric stress tensor is derived in terms the chain propagator, and is used to drive changes in cell shape according to a simple relaxation scheme. The method allows fully relaxed, stress-free configurations to be obtained, even in non-trivial morphologies, and enables the study of morphology transitions induced by external stresses.

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