Operator splitting boosts simulation efficiency

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Schematic of sliplink simulation for entangled polymers in shear flow



Snapshots from operator splitting simulation with increasing timestep (black, red, blue) demonstrates improved stability Many polymer dynamics simulations (e.g., sliplink models for entangled polymers in shear) are built on the Rouse model
Simulating the Rouse model is time-consuming

Approach:

Rouse model with noise and flow exactly solvable in terms of Rouse modes, allowing *arbitrary* timestep
Sliplink constraints, finite extensibility best handled in "real space"

• "Operator splitting": alternate steps of two evolution operators

Results:

Improved convergence over standard (explicit Euler) method
Improved stability: *much* larger timestep possible, 5—10x faster

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•Method applicable to broad class of simulations

of stochastic order parameters in flow

