Characterization of Chaotic Motion of DNA in Linear Shear Flows

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The chain does not change conformation under certain forces.

A chain whose conformation changes presumably enhances mixing.
Particle Simulation

- Forces
  - drag $F_D = -\zeta(\dot{r}_i - u_i)$
  - Brownian force (randomly directed)
  - spring force $F_S = k \frac{r_n - r_o}{1 - |r_o|^2/a^2}$

- Force values are normalized with fluid strain, so unique conditions can be identified with spring constant $k$ and drag coefficient $\zeta$

- For each time step, apply Newton’s law of motion. Time steps are small enough not to affect the solution.

- Bead location $r_i$ is collected for each time step for long periods of time, and statistics are collected.
Occasional Flip, $N = 3, \ k = 4, \ \zeta = 2.0,$

- Mode: Stable and stationary except for rare swapping of end beads.
Limit Cycle, $N = 3, \ k = 2.27, \ \zeta = 0.42$

- Mode: stable limit cycle with continuous motion (only two beads are shown)
Bifurcation, $N = 3$, $k = 1.07$, $\zeta = 0.52$

- Mode: 2 stable limit cycles where beads swap positions
Threshold, $N = 3$, $k = 2.27$, $\zeta = 1.07$

- Mode: Stable limit cycle on the threshold of switching to another mode.
Contact sheet
Conclusions

- Molecule conformation and dynamics can affect mixing.
- Different flow regimes can provide different levels of mixing due to chaos inherent to the dynamics.
- The motion of long chains is similar to short chains where the subchain motion propagates along the length.
- Chains in certain flow regimes mix better and possibly migrate due to chaotic motion.
- **Future work:** What are the effects of nonuniform shear flows and secondary forces on the dynamics of chains?
- **Future work:** Can knowledge of the dynamics yield better designs for DNA hybridization chambers by enhancing chaotic mixing?