Modeling Dynamics of Biological Filaments in Continuum Limit

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The 2017 Summer School on “Multibody System and Nonlinear Dynamics”
About me

• BTech. in Chemical Engineering (2012-16)
  - From IIT Guwahati
  - Computational/Experimental Fluid Dynamics

Montage photography club (https://www.facebook.com/montage.iitg/)

http://www.citiestips.com/city/GuwahatiIndia
Montage photography club (https://www.facebook.com/montage.iitg/)
About me

• Joined UC Merced in 2016
  – Water and Energy (WE Lab)
  – Bio-mechanics and Mechanobiology
Outline of the Presentation

• DPD
  – Introduction
  – Formulation
  – Results

• Rod Model
  – Introduction
  – Formulation
  – Results
Part I

Dissipative Particle Dynamics
A basic introduction to Meso-scale simulation
Multi-Scale Modeling

Based on SDSC Blue Horizon (SP3)
1.728 Tflops peak performance
CPU time = 1 week / processor

Atomistic Simulation Methods
- Ab initio methods
- Semi-empirical methods

Mesoscale methods
- Lattice Monte Carlo
- Brownian Dynamics
- Dissipative Particle Dynamics

Continuum Methods
- Monte Carlo (MC)
- Molecular Dynamics (MD)
- Tight-binding
  - MNDO, INDO/S

Time/s
- $10^0$
- (ns) $10^{-9}$
- (ps) $10^{-12}$
- (fs) $10^{-15}$

Length/m
- $10^{-10}$
- $10^{-9}$ (nm)
- $10^{-8}$
- $10^{-7}$
- $10^{-6}$ (μm)
- $10^{-5}$
- $10^{-4}$

F.R. Hung, K.E. Gubbins, and S. Franzen, Chemical Engineering Education, Fall 2004
Ab-initio

- Idea: Schrödinger equation is solved numerically
- Pros:
  - Can handle bond breaking/formation process
- Cons:
  - Only small system and fast processes

Semi-empirical

- Idea: Simplified versions of equations from ab initio methods (such as only valence electron)
- Pros:
  - Can handle larger system ($10^3$ atoms)
  - Longer times scale
- Cons:
  - Need experimental inputs and parameter sets
  - Non-transferable
**Molecular simulation**

- Idea: derived force field and sample atom configuration are used
- Pros:
  - Larger system
  - Longer time scale
- Cons:
  - Lose electronic properties, reaction

**Continuum Modeling**

- Idea: continuous; balance and constitutive equations
- Pros:
  - Macroscopic size and time scale
- Cons:
  - Molecular origin of behavior

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**DPD Rod Model**

UC Merced School of Engineering
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DPD(Meso Scale)

- Average out faster degree of freedom and/or treat large group of atoms as one particle
- Proposed by Hoogerbrugge and Koelman(1992) for simulating hydrodynamic behavior
- Pair forces of three types are involved
  - Conservative Force
  - Dissipative force
  - Stochastic(Random) force
Particles move according to Newton's equation of motion

\[
\frac{d\vec{r}_i}{dt} = \vec{v}_i; \quad \frac{d\vec{p}_i}{dt} = \vec{f}_i
\]

\[
\vec{r}_i \quad \text{position of particle } i
\]

\[
\vec{v}_i = \frac{\vec{p}_i}{m_i} \quad \text{velocity of particle } i
\]

\[
\vec{f}_i \quad \text{force on particle } i
\]

\[
m_i \quad \text{mass of particle } i
\]

Force is given by

\[
\vec{f}_i = \sum_{j \neq i} (\vec{f}_{ij}^C + \vec{f}_{ij}^D + \vec{f}_{ij}^R)
\]

Forces

- Conservative force comes from a simple potential with the form

\[ U(r_{ij}) = a_{ij}r_c \left(1 - \frac{r_{ij}}{r_c}\right)^2 \]

\[ f^C_{ij} = a_{ij} \left(1 - \frac{r_{ij}}{r_c}\right) \frac{\vec{r}_{ij}}{r_{ij}} \quad (r_{ij} < r_c) \]

\[ f^C_{ij} = 0 \quad (r_{ij} \geq r_c) \]

- \( \omega_d = \left(1 - \frac{r_{ij}}{r_c}\right) \)

- Is a “repulsion” parameter
- Is an interaction cut-off range parameter

\[ \vec{r}_{ij} = \vec{r}_i - \vec{r}_j; r_{ij} = |\vec{r}_{ij}| \]

Forces

• Dissipative forces is friction force that dissipates relative momentum (hence kinetic energy)

\[
\vec{f}_{ij}^{D} = -\gamma \omega_d (r_{ij}) (\hat{r}_{ij} \cdot \vec{v}_{ij}) \hat{r}_{ij}
\]

\(\vec{v}_{ij} = \vec{v}_i - \vec{v}_j\) is the relative velocity
\(\gamma\) is a friction coefficient
\(\omega_d\) is a distance dependent weight function that is zero for \(r_{ij} > r_c\)

Component of relative velocity along line of centres

Forces

• To have the correct canonical distribution, dissipative and random force are related

\[ \mathbf{f}_{ij}^R = -\sigma \omega_r (r_{ij}) \theta_{ij} \hat{r}_{ij} \]

- \( \sigma \) is a fluctuation amplitude
- \( \omega_r \) is a distance dependent weight function that is zero for \( r_{ij} > r_c \)
- \( \theta_{ij} \) is a Gaussian distributed random number with zero mean and unit variance
- \( \omega_d (r_{ij}) = \left[ \omega_r (r_{ij}) \right]^2 \)

• Modified velocity-verlet scheme can be defined as

\[
\begin{align*}
\vec{r}_i(t + \Delta t) &= \vec{r}_i(t) + \Delta t \vec{v}_i(t) + \frac{1}{2} \Delta t^2 \vec{f}_i(t) \\
\vec{v}'_i(t + \Delta t) &= \vec{v}_i(t) + \lambda \Delta t \vec{f}_i(t) \\
\vec{f}_i(t + \Delta t) &= \vec{f}_i(\vec{r}_i(t + \Delta t), \vec{v}_i'(t + \Delta t)) \\
\vec{v}_i(t + \Delta t) &= \vec{v}_i(t) + \frac{1}{2} \Delta t (\vec{f}_i(t) + \vec{f}_i(t + \Delta t))
\end{align*}
\]

Here \( \lambda \) is an adjustable parameter in the range 0-1.

Contact angle

• Angle measured through the liquid, where a liquid-vapor interface meets a solid interface

• Measurement techniques
  – Static Sessile drop method
  – Pendent drop method
  – Etc...

https://en.wikipedia.org/wiki/Contact_angle
Effect of curvature on contact angle

- Contact angle changes when the droplet is on a non-planer surface

Effect of curvature on contact angle
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Part II

Rod Model

Modeling of biological filaments in continuum limit
Modeling Bio-filaments in Continuum Limit Rod Model

Example Simulation Outputs


DNA structure at different scales

Length Scale (m)

- $10^{-9}$
- $10^{-8} - 10^{-7}$
- $10^{-7} - 10^{-5}$

[Calladine and Drew; Branden and Tooze; Nelson and Cox]
Formulation

• Characteristics in rod model
  – Deformation due to bending and
t  – Inertia and dissipation
  – Self contact
  – Drag and Non homogeneity

• Two reference frame
  – Body fixed
  – Inertial
Equation of rod dynamics

Linear Momentum Equation:

\[
\frac{\partial \vec{f}}{\partial s} + \vec{K} \times \vec{f} = m \left\{ \frac{\partial \vec{v}}{\partial t} + \vec{\omega} \times \vec{v} \right\} - \vec{F}
\]

Angular Momentum Equation:

\[
\frac{\partial \vec{Q}}{\partial s} + \vec{K} \times \vec{Q} = \vec{I} \cdot \frac{\partial \vec{\omega}}{\partial t} + \vec{\omega} \times \vec{I} \cdot \vec{\omega} + \vec{f} \times \vec{r} - \vec{Q}
\]
Equation of rod dynamics

Continuity of Cross-Section:

\[
\frac{\partial \vec{\omega}}{\partial s} + \vec{\kappa} \times \vec{\omega} = \frac{\partial \vec{\kappa}}{\partial t}
\]

\[
\frac{\partial \vec{\nu}}{\partial s} + \vec{\kappa} \times \vec{\nu} = \frac{\partial \vec{r}}{\partial t} + \vec{\omega} \times \vec{r}
\]

Constitutive law

\[
\vec{q}(s,t) = \vec{f}_n(\vec{\kappa}(s,t),...)
\]
Cross section Dynamics and Constitutive Law

\[ \vec{q}(s,t) = fn(\vec{\kappa}(s,t),...) \]

Restoring Torque

Curvature and Twist

\[ \frac{\partial \vec{a}_i}{\partial s} = \vec{\kappa} \times \hat{a}_i \]

Cross-section fixed reference frame \( \{\hat{a}_i(s,t)\} \)
Buckling analysis of a beam

• Using forward rod model, a cantilever beam was subjected to incremental load at the free end
• Linear constitutive law has been used

Figure 5 Elastic postbuckling curves for compressed elements

http://fgg-web.ffg.uni-lj.si/~/pmoze/ESDEP/master/wg06/l0300.htm
Conclusion

- DPD (Dissipative particle Dynamics) is a stochastic simulation techniques to simulate the rheological and dynamic properties of simple and complex fluid.
- The contact angle depends on the fluid and the surface properties.
- To simulate non-linear dynamics of biological filaments, Elastic rod model is a very useful and efficient tool.
- Constitutive law is an important parameter in modeling and lack of accurate information about it is a challenge.
State of the art
Thank you
Future Direction
Roadblock in the modeling

• Constitutive law is unknown for DNA

\[ \vec{q} = \vec{fn}(\vec{K},...) = ? \]

Restoring torque  Curvature and twist