Multicomponent Vesicles in Electric Fields

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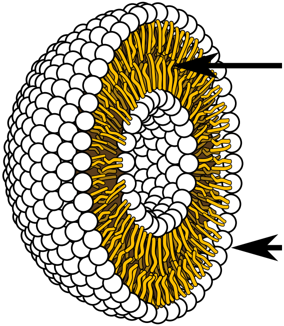
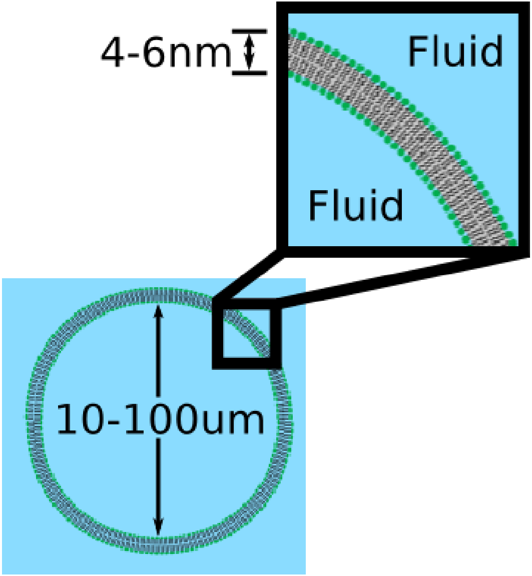
Vesicles



Hydrophobic Tails

Hydrophillic Heads

Vesicles



Vesicle Electrohydrodynamics

Courtesy of Salipante and Vlahovska

Multicomponent Vesicles: Three Components

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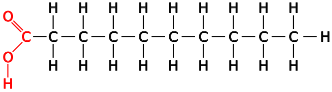

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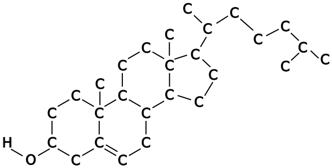
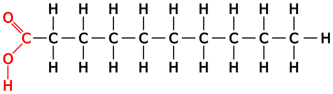


Cholesterol

Multicomponent Vesicles: Three Components



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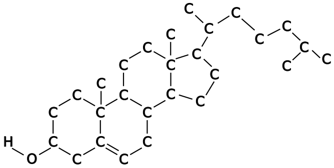

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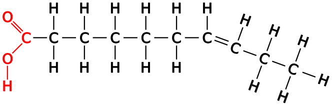
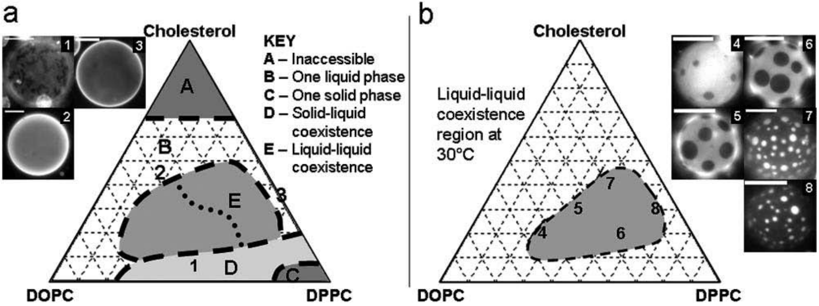


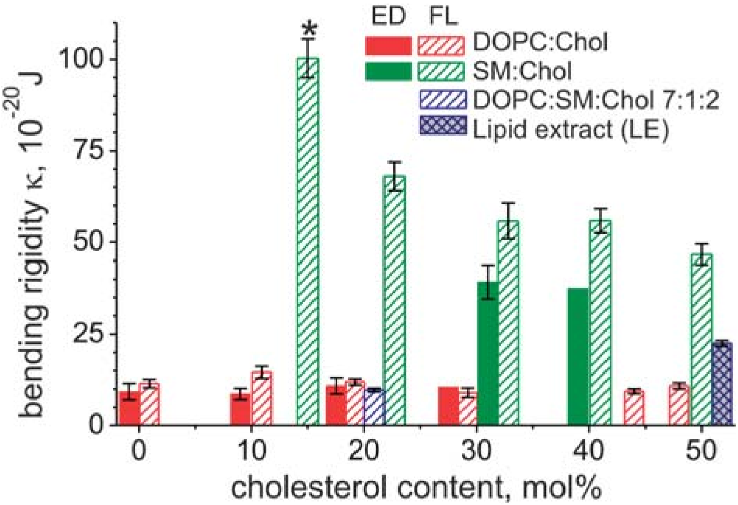
Unsaturated

Multicomponent Vesicles: Ternary Mixtures



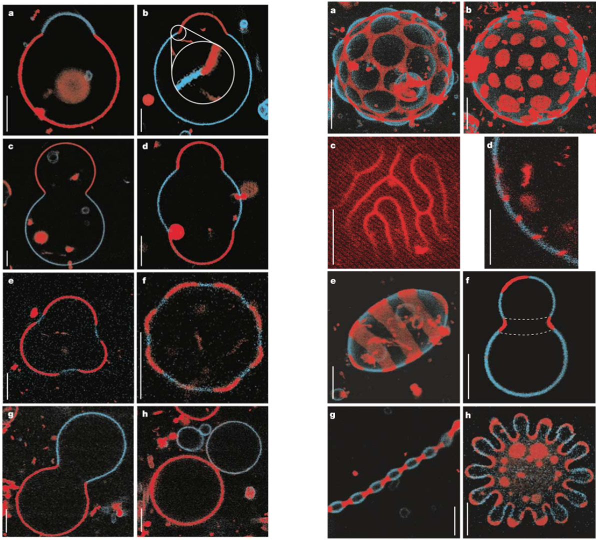
Veatch and Keller, Biophys J, 2003.

Multicomponent Vesicles: Variable Properties



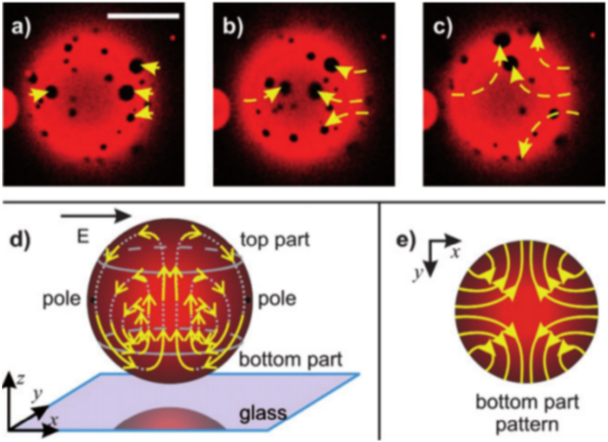
Gracia *et al*, Soft Matter, 2010.

Multicomponent Vesicle: Influence of Bending



Baumgart, Hess & Webb, Nature, 2003

Multicomponent Vesicle Electrohydrodynamics



Dimova *et al*, Soft Matter, 2009

Prior Modeling Works

- Electrohydrodynamics:
    1. McConnell, Miksis, and Vlahovska, IMA J Appl. Math, 2013
    2. Nganguia and Young, Phys. Rev. E, 2013
    3. Schwalbe, Vlahovska, and Miksis, Phys. Rev. E., 2011
    4. Yamamoto, Arand-Espinoza, Dimova, Liposky, Langmuir, 2010
    5. Others!
- Multicomponent:
    1. Liu, Marple, Allard, Li, Veerapaneni and Lowengrub, Soft Matter, 2017
    2. Yang, Du and Tu, Phys Rev E, 2017
    3. Li, Lowengrub and Voigt, Comm Math Sci, 2012
    4. Funkhouser, Solis, and Thornton, J Chem Phys, 2010
    5. Hu, Weikl and Lipowsky, Soft Matter, 2011
    6. Sohn, Tseng, Li, Voigt, and Lowengrup, J Comp Phys, 2010
    7. Others!

Goal

To model the dynamics of both 2D and 3D multi-component vesicles with varying fluid and membrane properties in the presence of electric fields.

Outline

1. Introduction
2. General Modeling Framework
3. Aside: Justification for Navier-Stokes
4. Multi-Component Electrohydrodynamics

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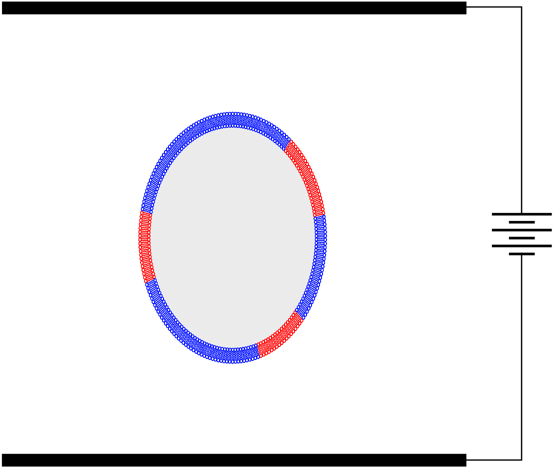
System of Interest



Some Basics

- Impermeable Membrane
    - Conserved inner volume
    - Ions can not pass through membrane without nano/macro pores.

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- Membrane resists bending
- Trans-Membrane Potential: V_m
  - Time-evolving
  - Discontinuous electric potential field

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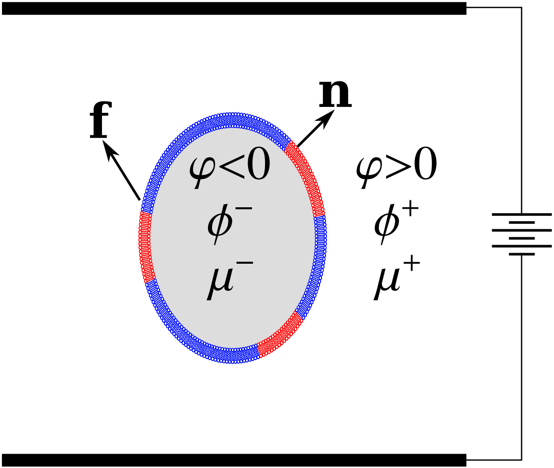

Constitutive/Energy Equations

Total Energy

$$E = E_b + E_K + E_\gamma + E_q + E_V$$

E_b: Total Bending

$$E_b = \int_\Gamma \frac{\kappa_c}{2} (H - c_0)^2 \ \mathrm{dA}$$

E_K: Gaussian Bending

$$E_K = \int_\Gamma k_g K \ \mathrm{dA}$$

E_γ: Tension

$$E_\gamma = \int_\Gamma \gamma \ \mathrm{dA}$$

E_q: Phase

$$E_q = \int_\Gamma \left(g + \frac{\epsilon^2}{2} \|\nabla q\|^2 \right) \ \mathrm{dA}$$

E_V: Capacitance

$$E_V = \int_\Gamma \frac{C_m}{2} V_m^2 \ \mathrm{dA}$$

Constitutive/Energy Equations: Dependence on q

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Electric Potential Field (Leaky Dielectric)

Electric Potential Field

$$\nabla^2 \phi^{in,out} = 0$$

Potential Jump

$$\phi^{out} - \phi^{in} = -V_m$$

Electric Field

$$\boldsymbol{E}^{in,out} = -\nabla \phi^{in,out}$$

Normal Electric Field

$$\boldsymbol{n} \cdot \left(s^{out} \boldsymbol{E}^{out} - s^{in} \boldsymbol{E}^{in} \right) = 0$$

Trans-Membrane Potential

$$C_m \frac{DV_m}{Dt} + G_m V_m = \boldsymbol{n} \cdot \left(s^{out} \boldsymbol{E}^{out} \right) = \boldsymbol{n} \cdot \left(s^{in} \boldsymbol{E}^{in} \right)$$

Phase Evolution Relations

Phase Chemical Potential

$$\mu = \frac{\delta E}{\delta q}$$

Conserved Phase Evolution

$$\frac{Dq}{Dt} = \nabla_s \cdot (\nu \nabla_s \mu)$$

Fluid Relations

Fluid Momentum

$$\rho \frac{D\boldsymbol{u}}{Dt} = \nabla \cdot \boldsymbol{\sigma}$$

Fluid Stress Tensor

$$\boldsymbol{\sigma} = -p\boldsymbol{I} + \mu \left(\nabla \boldsymbol{u} + \nabla^T \boldsymbol{u} \right)$$

Area/Volume Conservation

$$\nabla_s \cdot \boldsymbol{u} = 0 \text{ on } \Gamma$$

$$\nabla \cdot \boldsymbol{u} = 0 \text{ in } \Omega$$

Maxwell Stress Tensor

$$\boldsymbol{\sigma}_E = \varepsilon \left(\boldsymbol{E} \otimes \boldsymbol{E} - \frac{\boldsymbol{E} \cdot \boldsymbol{E}}{2} \boldsymbol{I} \right)$$

Fluid Interface Balance

$$\boldsymbol{u}^{out} - \boldsymbol{u}^{in} = \boldsymbol{0}$$

$$\left(\boldsymbol{\sigma}^{out} - \boldsymbol{\sigma}^{in} \right) \cdot \boldsymbol{n} + \left(\boldsymbol{\sigma}_E^{out} - \boldsymbol{\sigma}_E^{in} \right) \cdot \boldsymbol{n} = \boldsymbol{f} = -\frac{\delta E}{\delta \Gamma}$$

Assumptions/Simplifications

- No spontaneous curvature: $c_0 = 0$
- Constant Gaussian Rigidity: $k_g =$Constant
- Tension enforces $\nabla_s \cdot \boldsymbol{u} = 0$: No explicit dependence on q
- All terms of $fH\boldsymbol{n} - \nabla_s f$ are added to tension

Variations

- Interface Variation:

$$\begin{aligned}\frac{\delta E}{\delta \Gamma} = &-\frac{k_c}{2}\, H\left(H^2 + 2K\right)\boldsymbol{n} - k_c\boldsymbol{n}\nabla_s^2 H - \nabla_s\gamma + \gamma H\boldsymbol{n} \\ &- \frac{1}{2}H^2\nabla_s k_c - H\boldsymbol{n}\nabla_s^2 k_c \\ &- \epsilon^2\left(\nabla_s q\cdot\boldsymbol{L}\nabla_s q\right)\boldsymbol{n} + \frac{\epsilon^2}{2}\|\nabla_s q\|^2 H\boldsymbol{n} + \epsilon^2\left(\nabla_s q\right)\nabla_s^2 q\end{aligned}$$

- Phase Variation:

$$\frac{\delta E}{\delta q} = \frac{dg}{dq} - \epsilon^2\nabla_s^2 q + \frac{1}{2}\frac{dk_c}{dq}H^2 + \frac{1}{2}\frac{dC_m}{dq}V_m^2$$

Non-Dimensional Equations

- Fluid Momentum:

$$\begin{aligned}\rho\frac{D\boldsymbol{u}}{Dt} = &-\nabla p + \frac{1}{\mathrm{Re}}\nabla\cdot\left[\mu(\phi)\left(\nabla\boldsymbol{u}+\nabla^{T}\boldsymbol{u}\right)\right] \\ &+ \delta(\phi)||\nabla\phi||\left(\nabla_{s}\gamma-\gamma H\boldsymbol{n}\right) \\ &+ \frac{\delta(\phi)}{\mathrm{Re}}\|\nabla\phi\|\left(\frac{1}{\mathrm{Ca}}\boldsymbol{f}_{bending}+\frac{1}{\alpha\mathrm{Ca}}\boldsymbol{f}_{spf}+\mathrm{Mn}\boldsymbol{f}_{electric}\right)\end{aligned}$$

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- Surface Phase:

$$\begin{aligned}\frac{Dq}{Dt} =& \frac{1}{\mathrm{Pe}}\nabla_s\cdot\left(\nu\nabla_s\mu\right)\\ \mu =& \frac{dg}{dq}-\mathrm{Cn}^2\nabla_s^2 q+\frac{\mathrm{Cn}^2}{2}\left(\alpha\frac{dk_c}{dq}H^2+\beta\frac{dC_m}{dq}V_m^2\right)\end{aligned}$$

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- Trans-membrane Potential:

$$C_{m}\frac{dV_{m}}{dt}+G_{m}V_{m}=\boldsymbol{n}\cdot\left(s^{out}\boldsymbol{E}^{out}\right)=\boldsymbol{n}\cdot\left(s^{in}\boldsymbol{E}^{in}\right)$$

General Simulation

General Steps

1. Initialize grid and initial level set function.
2. Update trans-membrane potential and electric field.
3. Update fluid velocity, pressure, and tension.
4. Advect level set and surface quantities.
5. Update surface phases.
6. Go to step 2.

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Additional Information

- Each individual component is tested and convergence properties investigated.
- Time step analysis ensures that the entire simulation has converged to a solution.

Numerical Method References

- Level Set Method: Velmurugan, Kolahdouz & DS (CMAME, 2016)
- Navier-Stokes Projection Method: DS & Miksis (JCP, 2011), Kolahdouz & S (JCP, 2015), DS (CPC, 2016)
- Trans-Membrane Potential: Kolahdouz & DS (AML, 2015)
- Single-Component Vesicle Electrohydrodynamics: Kolahdouz & DS (JCP, 2015), Kolahdouz & DS (PRE, 2015)
- Multi-Component Vesicle Dynamics: Gera & DS (C&F, 2018), Gera & DS (Soft Matter, In Review)
- Multi-Component Vesicle Electrohydrodynamics: Working on it!

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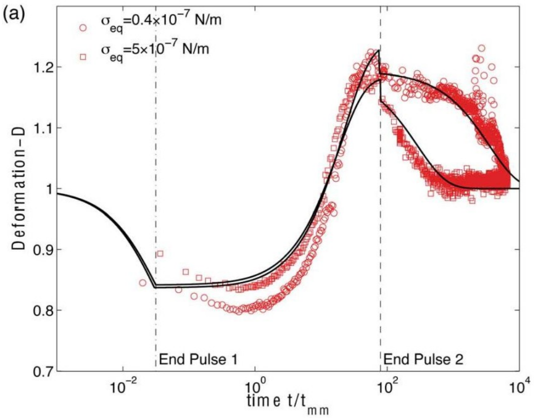
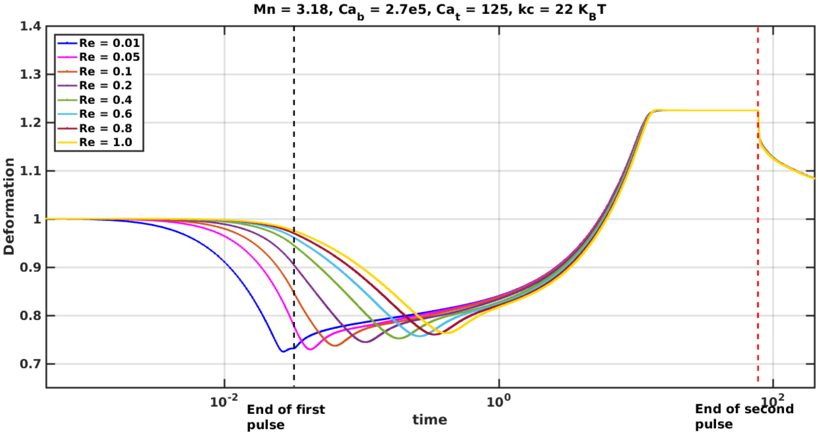
Experimental EHD

Stokes vs Experimental EHD



Salipante and Vlahovska, Soft Matter, 2014

Computational EHD with inertia



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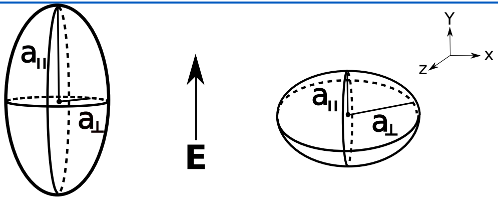
Prolate vs Oblate



Prolate elongated shape ($D=a_{\parallel}/a_{\perp}>1$) Oblate flat shape ($D=a_{\parallel}/a_{\perp}<1$)

Expectations

- Inner fluid less conductive than outer fluid ($\lambda < 1$): Prolate→Oblate→ Prolate
- Inner fluid more conductive than outer fluid ($\lambda > 1$): Prolate→Prolate
- The oblate-prolate transition occurs around the membrane charging time
- Require minimum electric field strength to achieve POP.

Single Component Prolate-Oblate-Prolate

Sub-critical E-Field: No POP

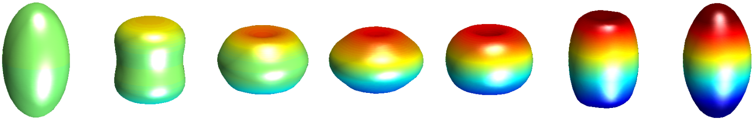
Colors indicate membrane voltage.

Super-critical E-Field: POP

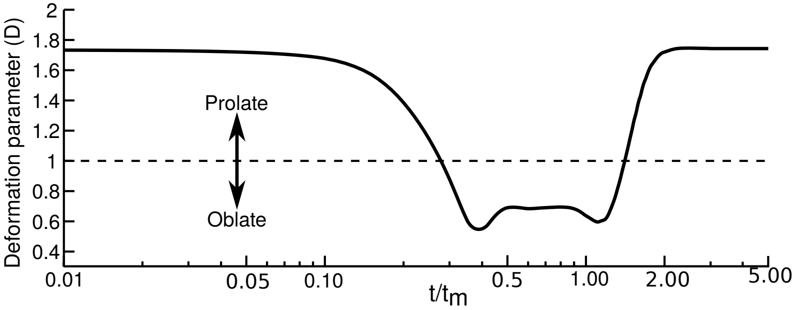
Colors indicate membrane voltage.

Evolution of Deformation Parameter ($D = a_{\parallel}/a_{\perp}$)

Sample Deformation



Deformation Parameter Over Time



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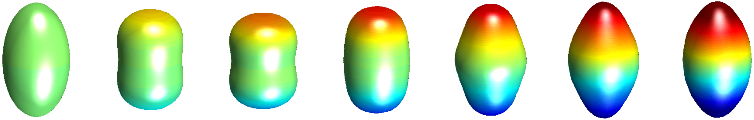

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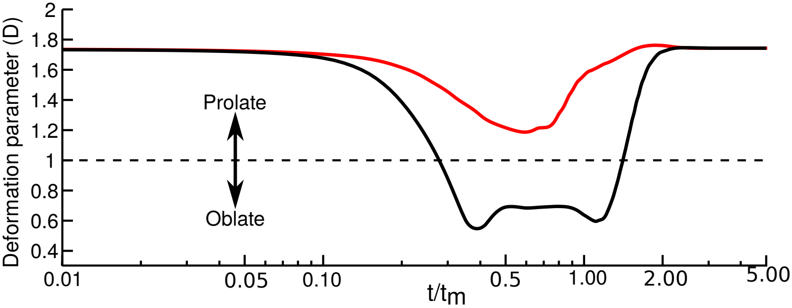
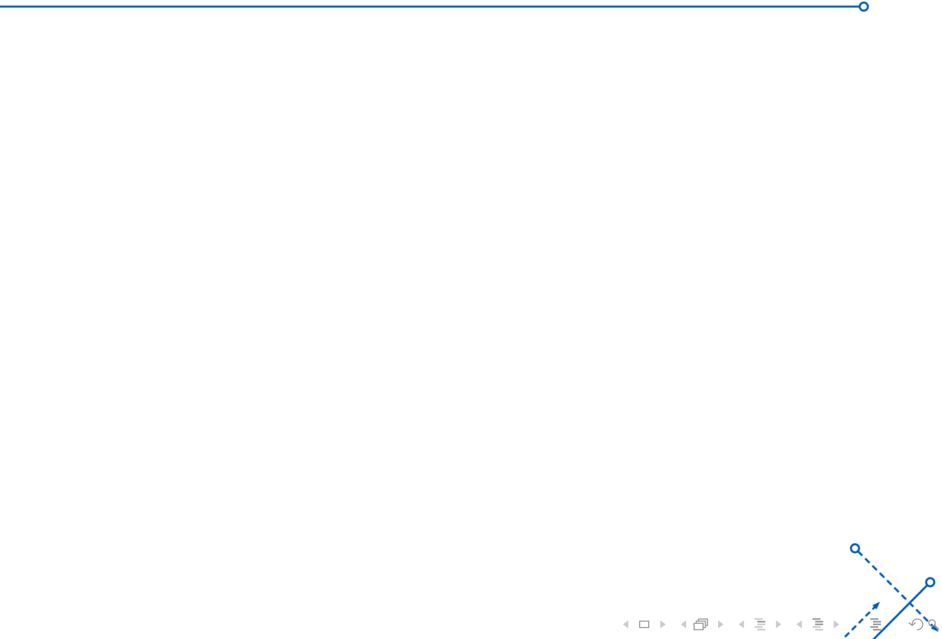


Common Parameters

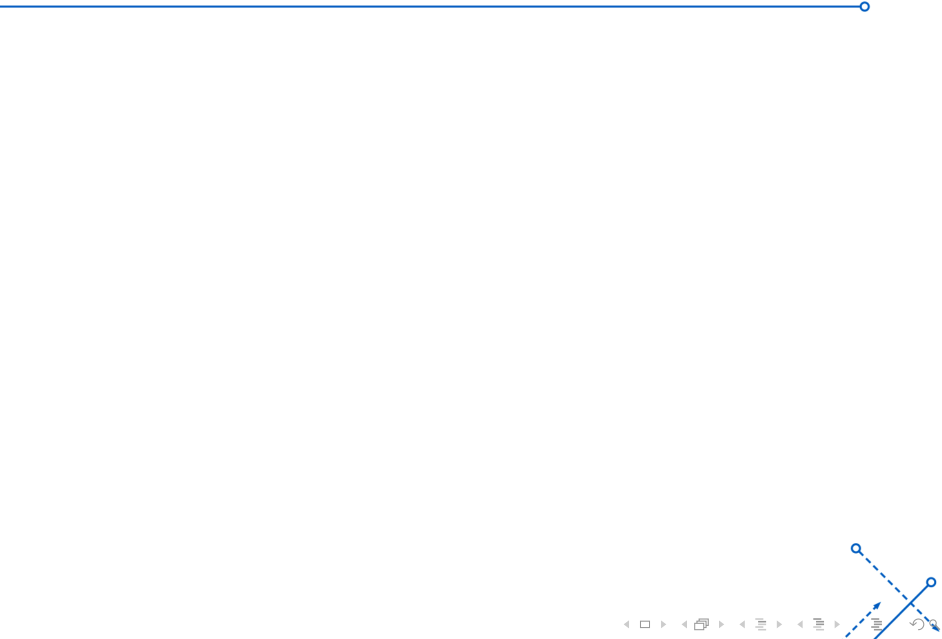
- Reduced Volume = 0.9 (3D) and Reduced Area = 0.85 (2D)
- $\bar{q} = 0.4$
- $\mathrm{Mn} = 20$
- $\beta = 10$
- $\mathrm{Ca} = 1$
- $\mathrm{Pe} = 1$
- $\nu = 1$
- $\mathrm{Re} = 0.1$
- $\lambda = s^{in}/s^{out}$
- Matched Viscosity
- Matched Bending Rigidity
- Properties will be (blue, red)

Multi-Component Prolate-Oblate-Prolate

$\lambda = 0.1,\ C_m = (0.2, 0.1),\ G_m = (0, 0)$

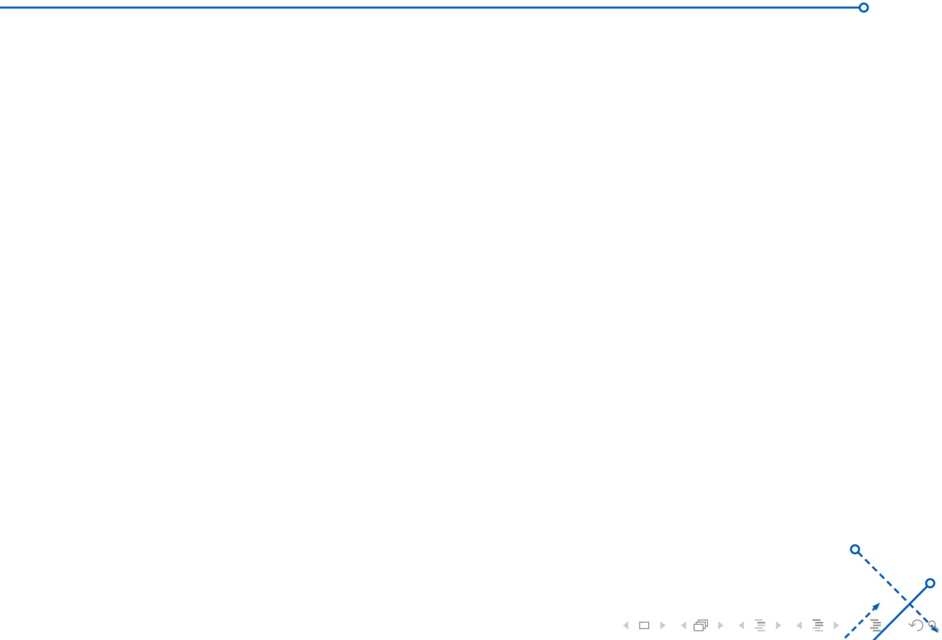


$\lambda = 0.1,\ C_m = (0.2, 0.1),\ G_m = (0.5, 0)$

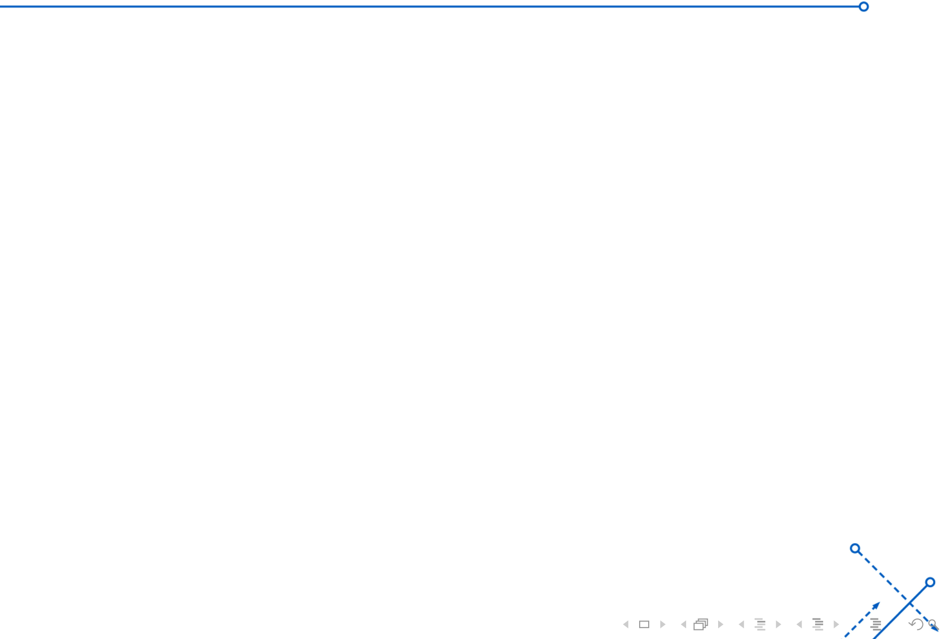


Multi-Component Prolate-Prolate

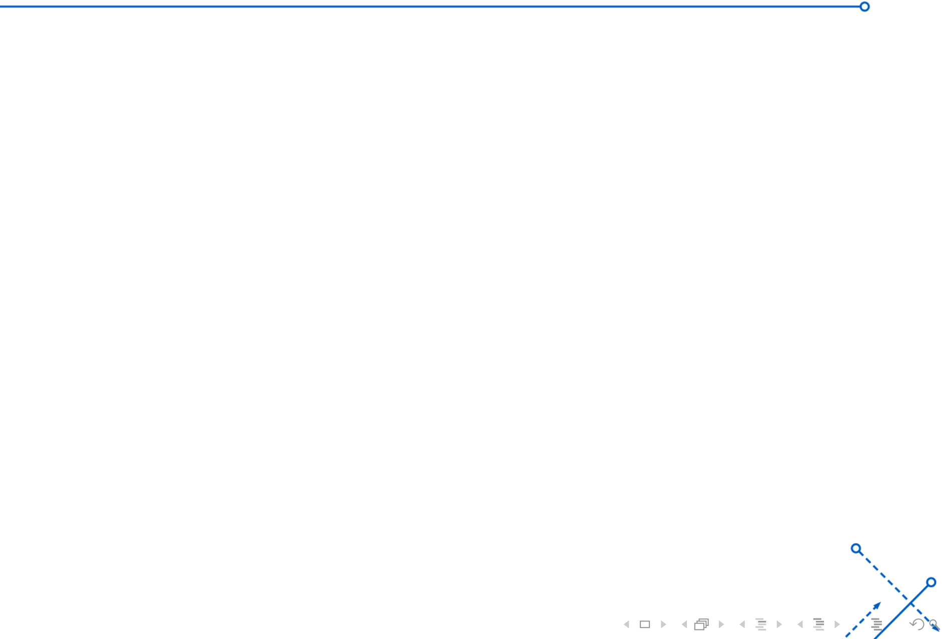
$\lambda = 10,\ C_m = (0.2, 0.2),\ G_m = (0, 1)$



$\lambda = 10,\ C_m = (0.2, 0.2),\ G_m = (1, 0)$



$\lambda = 10,\ C_m = (0.4, 0.2),\ G_m = (0, 0)$



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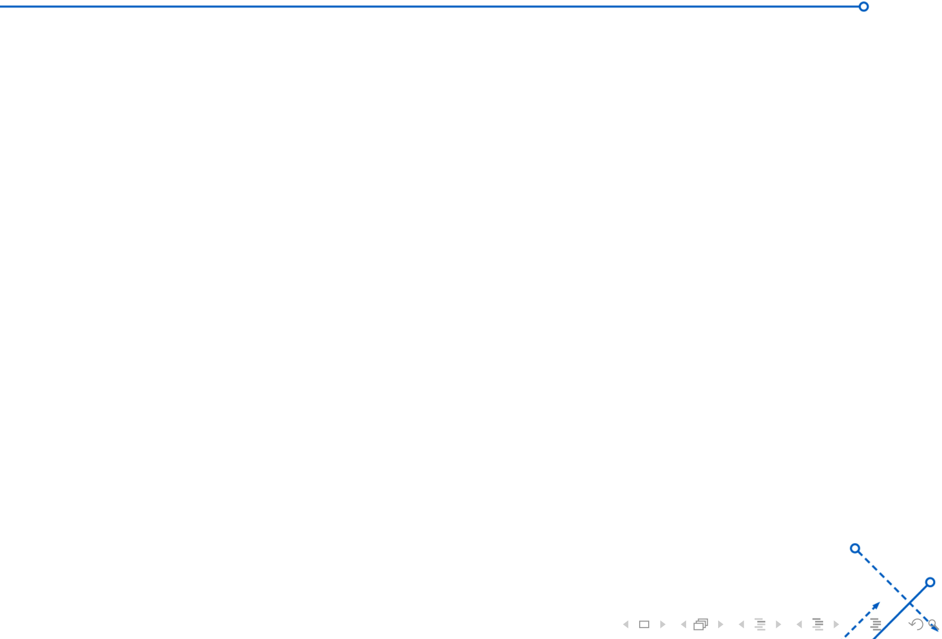


$\lambda = 10,\ G_m = (0, 0)$

$C_m = (0.4, 0.2)$

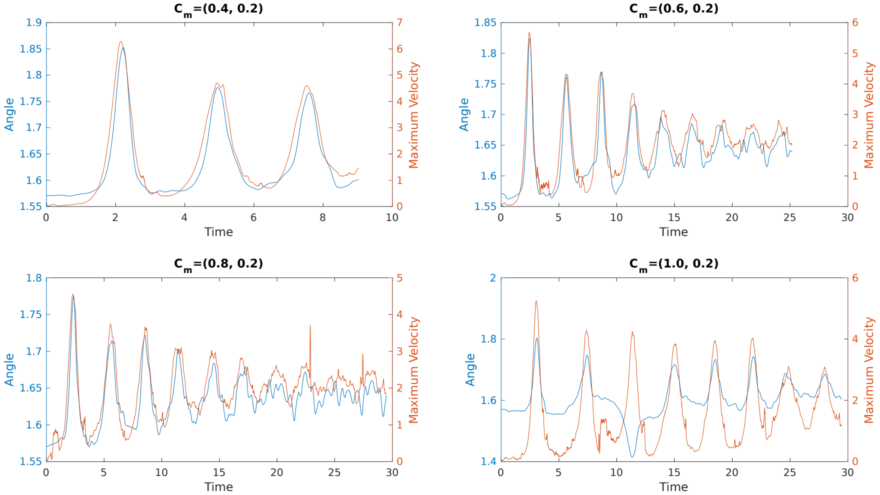
$C_m = (0.6, 0.2)$

$\lambda = 10, \; G_m = (0, 0)$

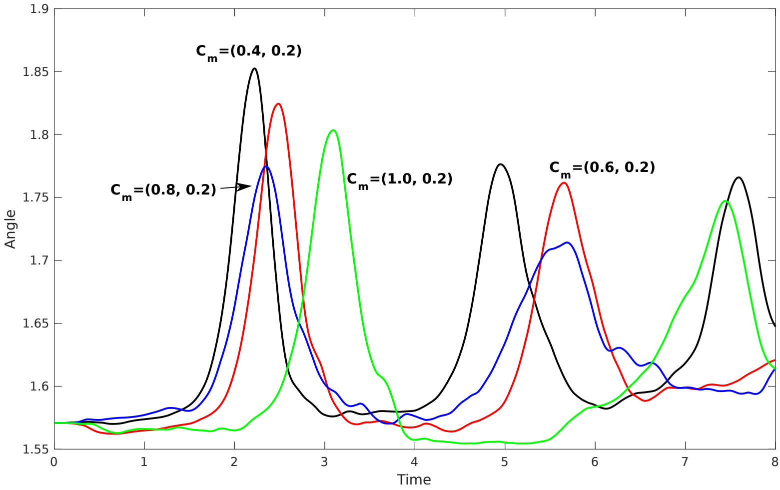
$C_m = (0.8, 0.2)$

$C_m = (1.0, 0.2)$

Inclination Angle & Maximum Velocity

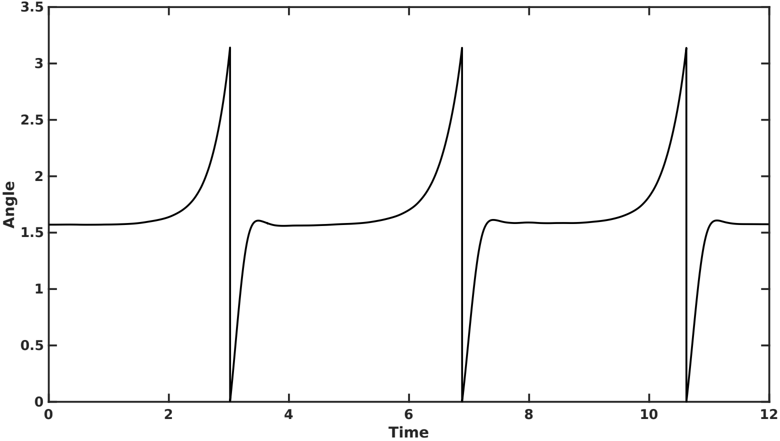


Inclination Angle



Large Inner Viscosity ($\nu = 10$)

$\nu = 10$ Inclination Angle



Many Vesicle Simulations

$\lambda = 0.1$: High Density

$\lambda = 0.1$: Low Density

$\lambda = 10$: High Density

$\lambda = 10$: Low Density

Final Comments

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Thanks and Questions

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