The Role of Adhesion in Vesicle Suspensions

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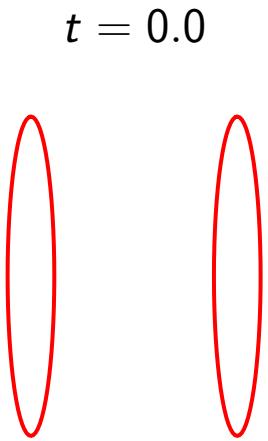
Outline

- Vesicle Suspensions with Adhesion
- Numerical Methods
- Adhesion in Stationary Flows
- Adhesion in Shear Flows
- Concluding Remarks



Vesicle Suspensions

Stokesian flow

$$\Delta \mathbf{v} = \nabla p \qquad \mathbf{x} \in \Omega$$
$$\nabla \cdot \mathbf{v} = 0 \qquad \mathbf{x} \in \Omega$$
$$\nabla_\gamma \cdot \mathbf{v} = 0 \qquad \mathbf{x} \in \gamma$$

Boundary conditions

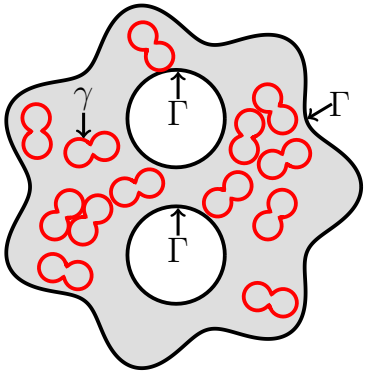
$$\mathbf{v} = \mathbf{f} \qquad \mathbf{x} \in \Gamma$$
$$[\![-pI + (\nabla \mathbf{v} + \nabla \mathbf{v}^T)]\!]\mathbf{n} = \mathbf{f} \qquad \mathbf{x} \in \gamma$$

Traction jump

$\mathbf{f}$ models resistance to bending and stretching, and **adhesion**

Bending and Strecthing

$$\mathbf{f}_B = k_b \int_\gamma \kappa^2 ds_y, \quad \mathbf{f}_T = \int_\gamma \sigma ds_y$$



Adhesion Model

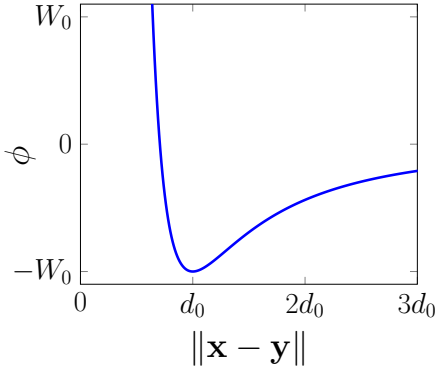
Sukumaran and Seifert, PRE 2001

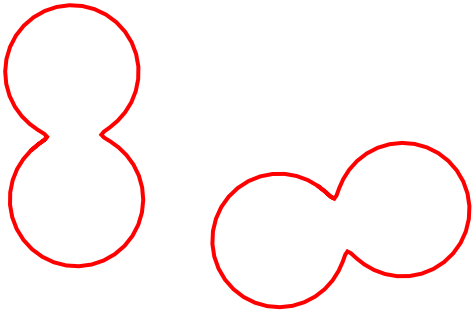
Adhesion potential

$$\phi(z) = W \left(\frac{d_0}{z}\right)^2 \left[\left(\frac{d_0}{z}\right)^2 - 2\right]$$

Adhesion force

$$\mathbf{f}_A(\mathbf{x}) = \nabla \int_\gamma \phi(\|\mathbf{x} - \mathbf{y}\|) ds_{\mathbf{y}}, \quad \mathbf{x} \notin \gamma$$





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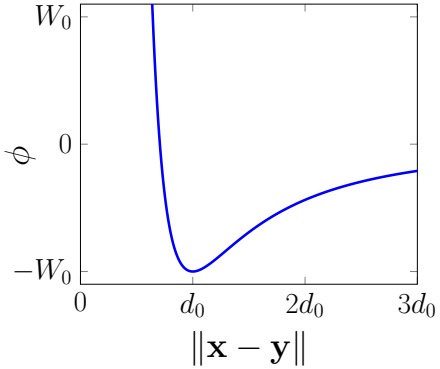

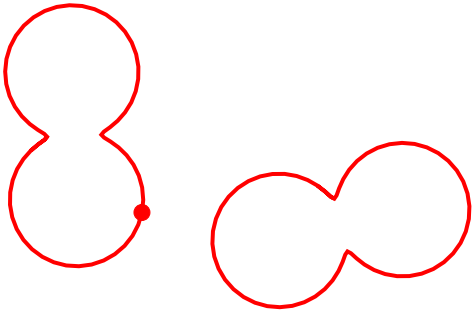

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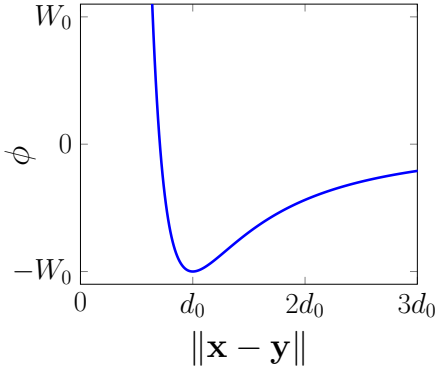

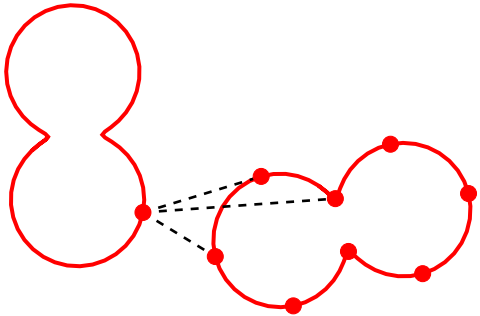

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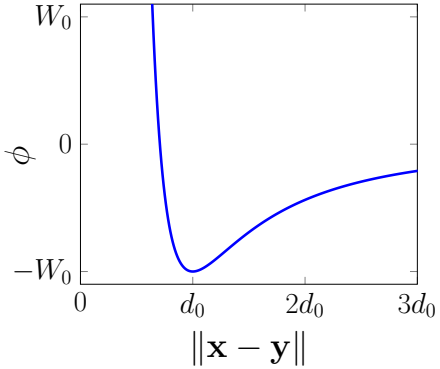

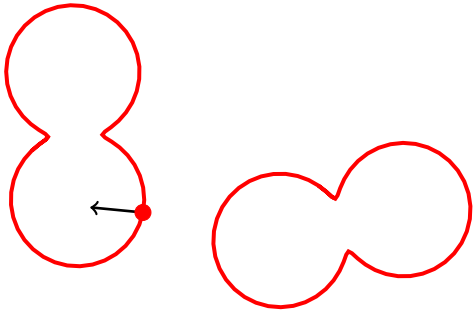

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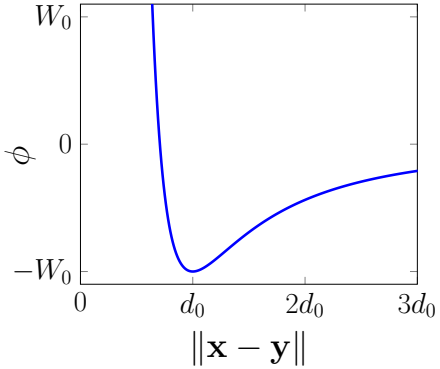

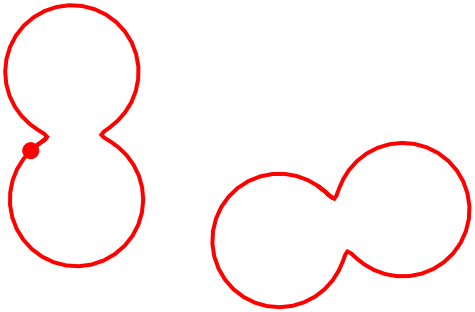

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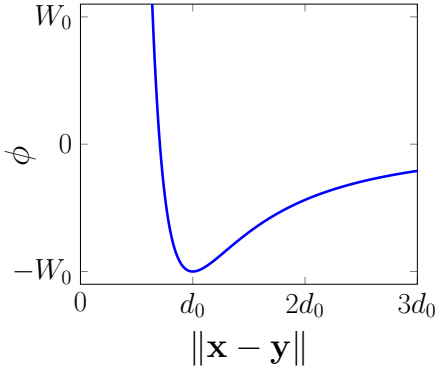

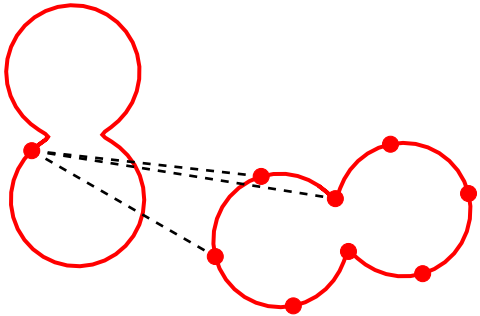

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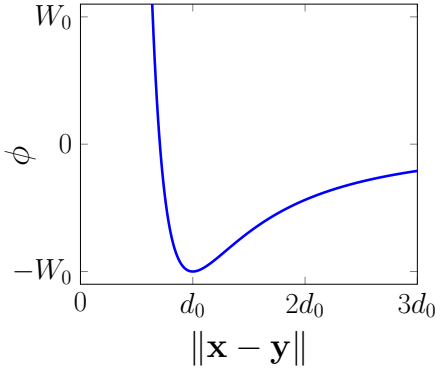

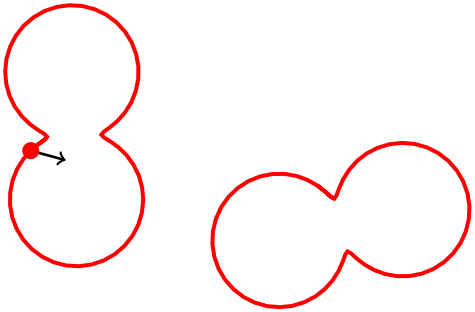

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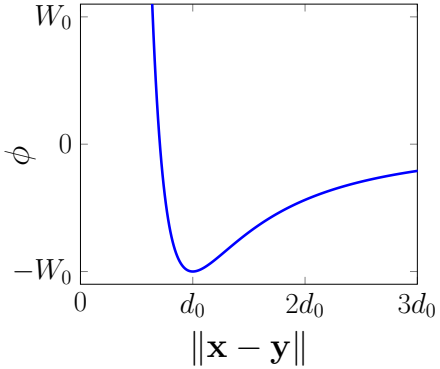
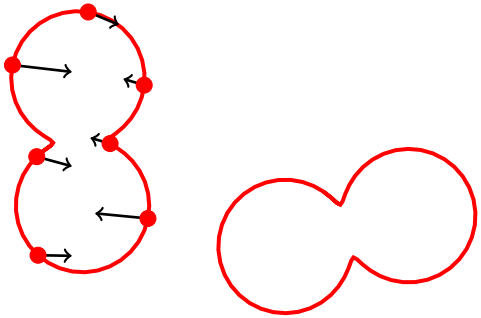
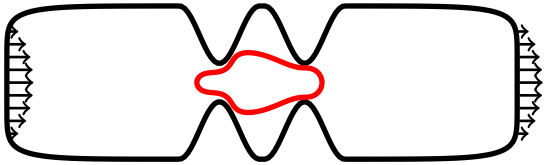




Governing Equations



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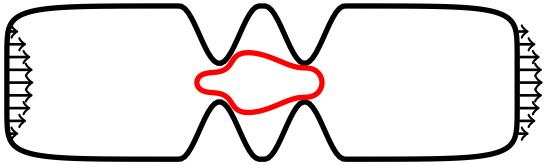

Fluid equations

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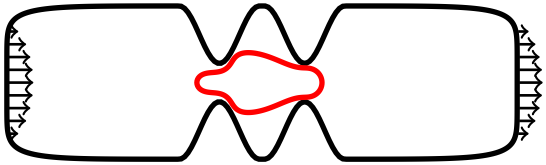

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$$\mathbf{v} \to 0 \qquad |\mathbf{x}| \to \infty$$
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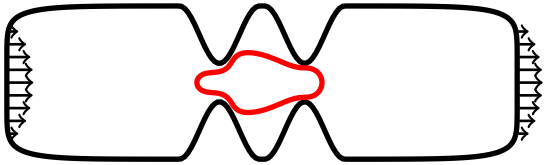

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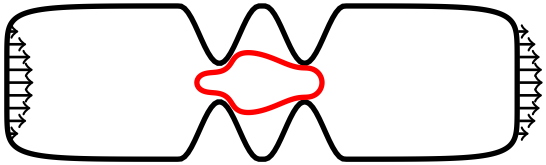
Vesicle force

$$\mathbf{f}(\mathbf{x}, \sigma) = \mathbf{f}_B + \mathbf{f}_T + \mathbf{f}_A$$

Governing Equations



Vesicle equations

$$\frac{d\mathbf{x}}{dt} = \mathcal{S}[\mathbf{f}] \qquad \mathbf{x} \in \gamma$$
$$0 = \nabla_\gamma \cdot \mathcal{S}[\mathbf{f}] \qquad \mathbf{x} \in \gamma$$

Stokes single-layer potential

$$\mathcal{S}[\mathbf{f}] = \frac{1}{4\pi} \int_\gamma \left(-\log \rho + \frac{\mathbf{r} \otimes \mathbf{r}}{\rho^2} \right) \mathbf{f}(\mathbf{y}) ds_{\mathbf{y}}$$

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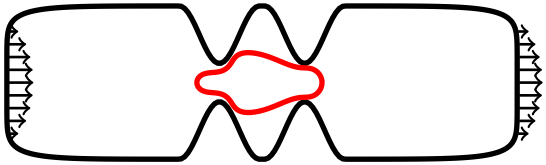

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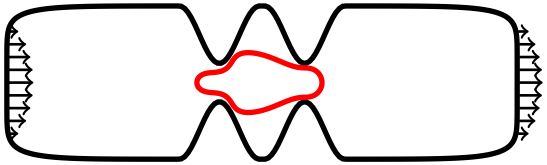

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Nyström method

$$\mathcal{S}[\mathbf{f}](\mathbf{x}) \approx \sum_k w_k G_S(\mathbf{x}, \mathbf{x}_k)\mathbf{f}_k$$

Spectral representation

$$\mathbf{x}(\theta, t) = \sum_n \hat{\mathbf{x}}_n(t) e^{in\theta}$$

$$\sigma(\theta, t) = \sum_n \hat{\sigma}_n(t) e^{in\theta}$$

Fourier differentiation

$$\frac{d\sigma}{d\theta} = \sum_n in\hat{\sigma}_n(t) e^{in\theta}$$

Trapezoid Rule

$$\int_\gamma \phi(\mathbf{x}) ds_{\mathbf{x}} = \sum_{n=1}^{N} w_n \phi(\mathbf{x}_n)$$

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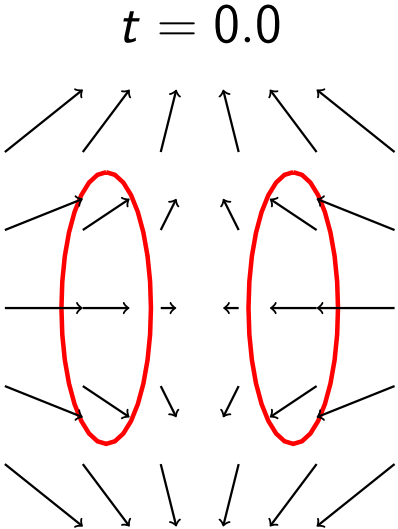
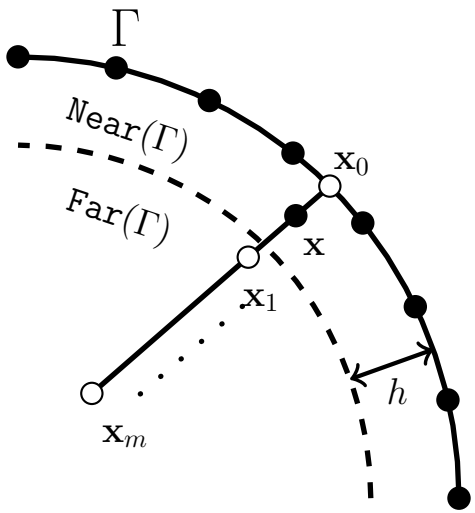
Extensional Flow





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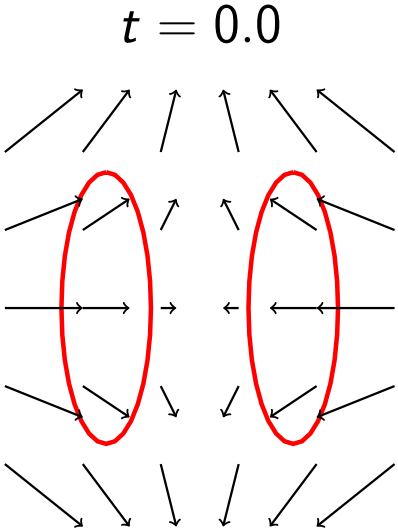
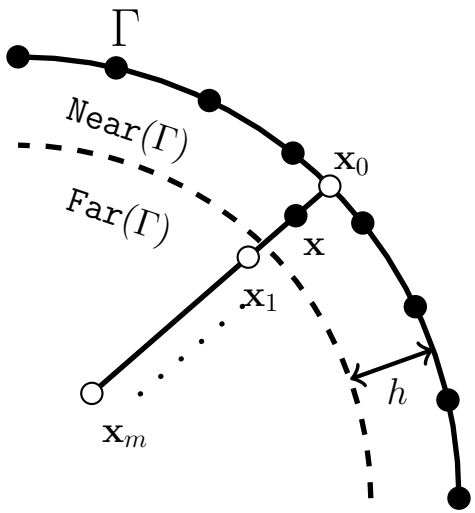
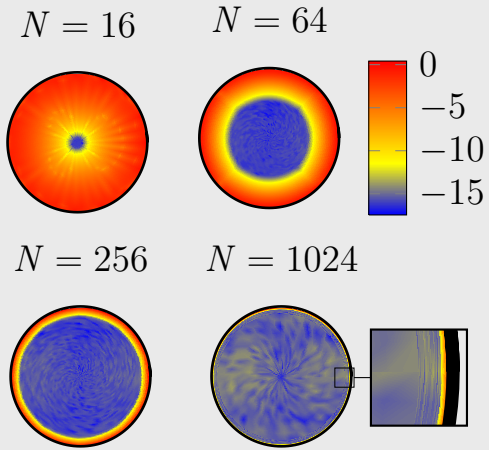




Near-Singular Integration

Q. and Biros, JCP 2014

Trapezoid Error



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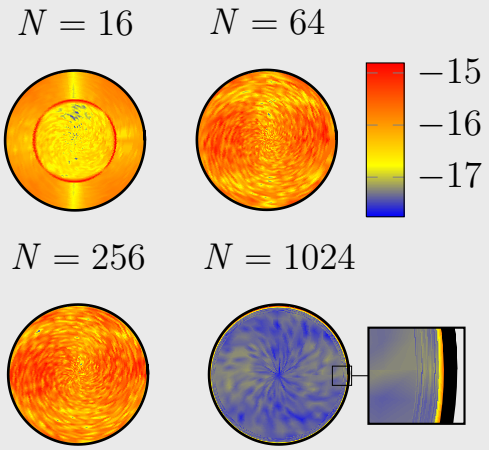
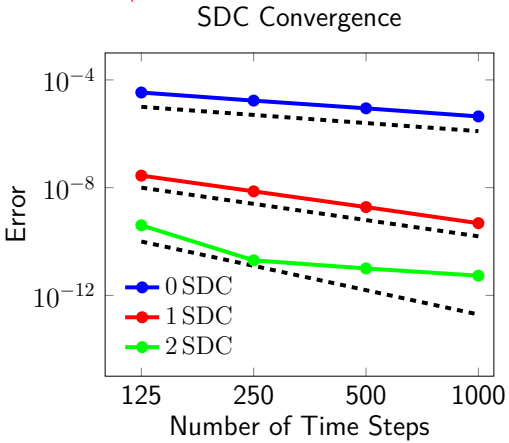


Spectral Deferred Correction

Q. and Biros, JCP 2016



$$\frac{\mathbf{x}^{N+1} - \mathbf{x}^N}{\Delta t} = \mathbf{v}[\mathbf{x}^{N+1}]$$

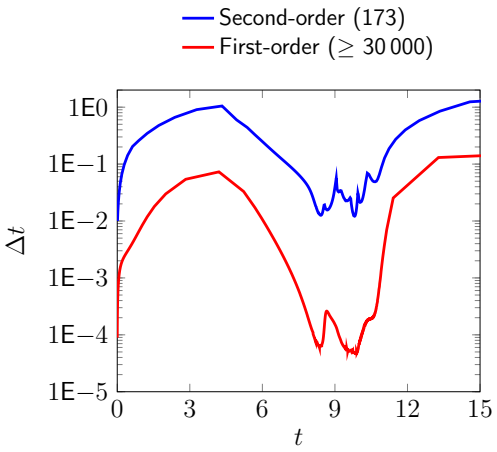
$$\mathbf{r}(\mathbf{x}) = \mathbf{x}^{N+1} - \mathbf{x}^N + \int_{t^N}^{t^{N+1}} \mathbf{v}[\mathbf{x}] d\tau$$

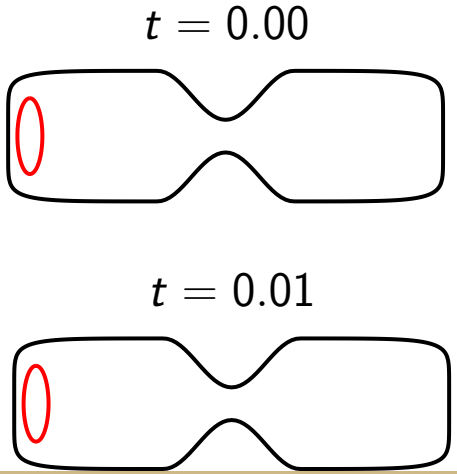
$$\frac{\mathbf{e}^{N+1} - \mathbf{e}^N}{\Delta t} = \mathbf{r} + \mathbf{v}[\mathbf{x}^{N+1} + \mathbf{e}^{N+1}]$$

- Residual is approximated with quadrature
- Substeps used to achieve high-order

Adaptive Time Stepping

- Crucial for problems with multiple time scales
- Local truncation error estimated with area and length





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Relaxation with Adhesion

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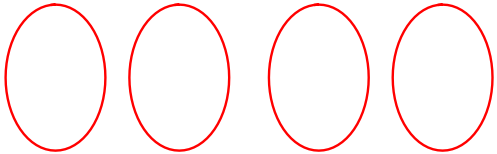

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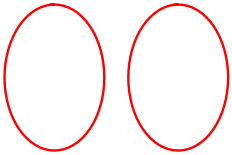
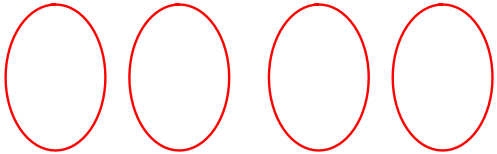
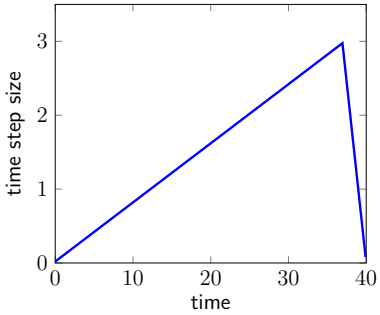
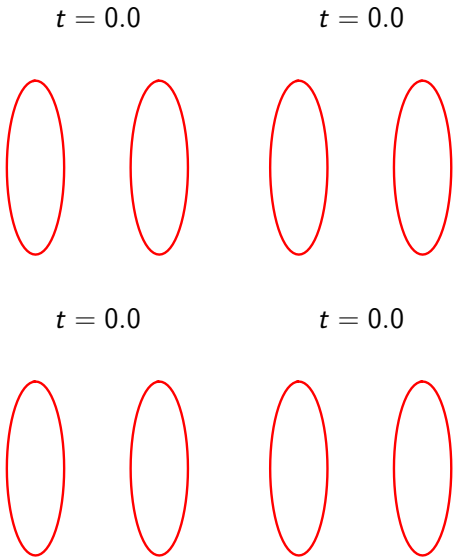


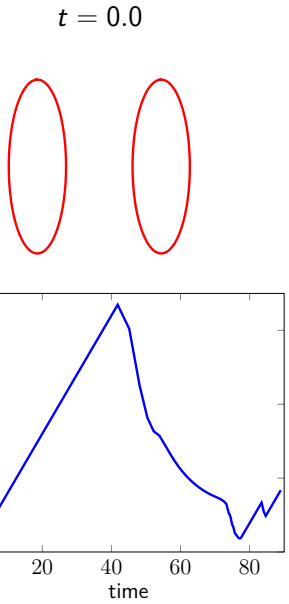
$t = 0.0$ $t = 0.0$



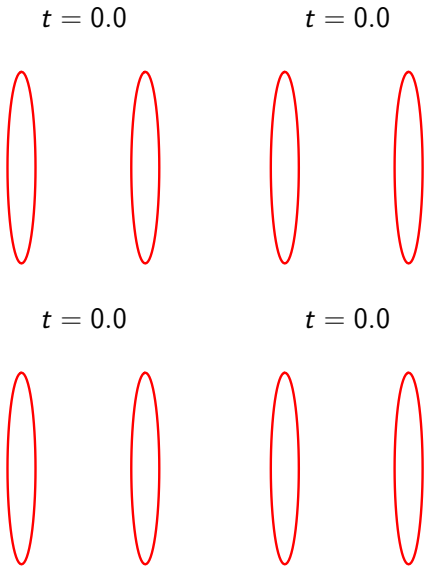


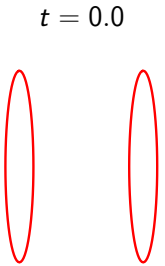
Relaxation with Adhesion

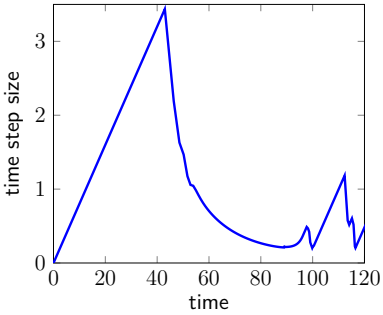




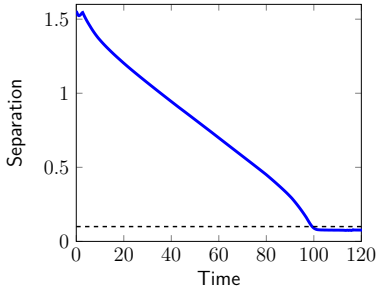
Relaxation with Adhesion

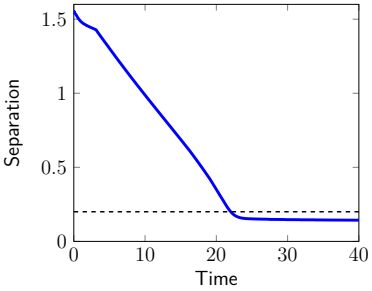


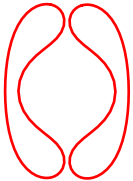


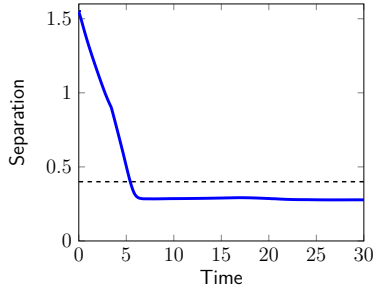


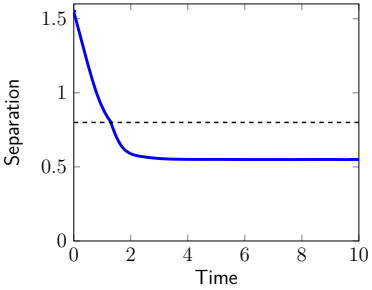
Minimum Separation

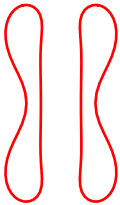




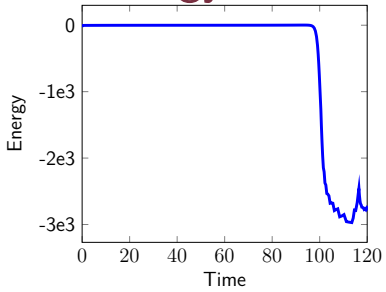


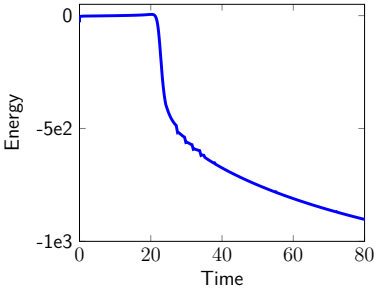


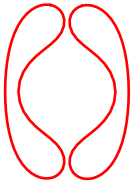


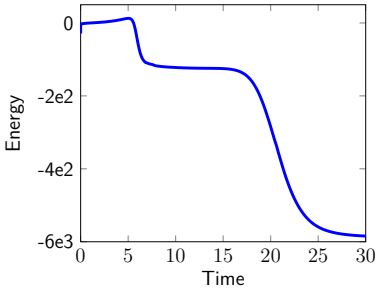


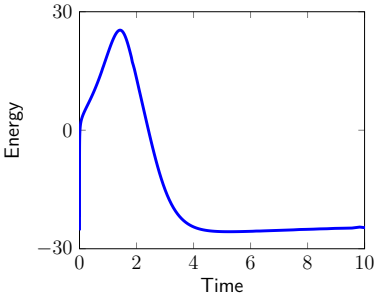
Total Energy

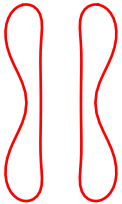






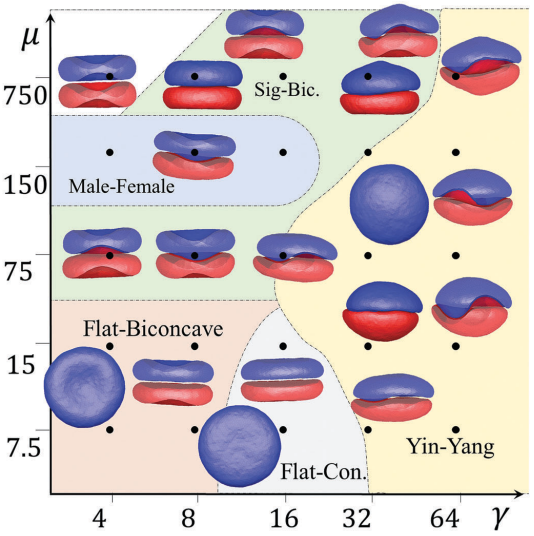






Doublets in $\mathbb{R}^3$

Hoore et al, Soft Matter, 2018

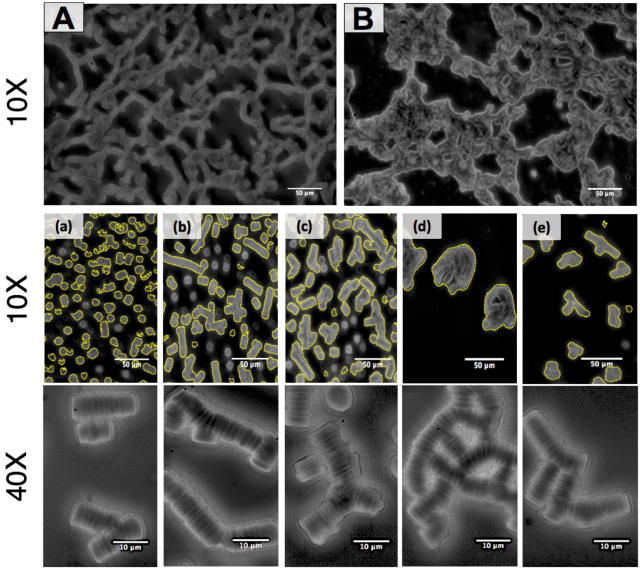


- Adhesion between closest vertices
- Lennard-Jones 12-6 potential
- γ is the adhesion strength
- μ is the shear modulus
- Reduced volume is 0.64

Outline

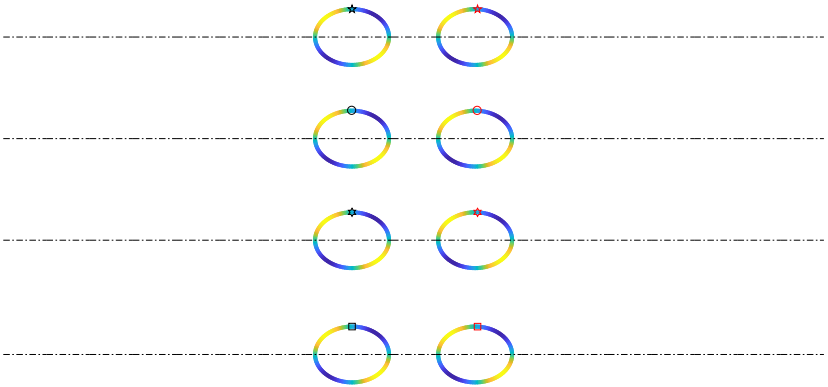
- Vesicle Suspensions with Adhesion
- Numerical Methods
- Adhesion in Stationary Flows
- **Adhesion in Shear Flows**
- Concluding Remarks

Aggregates of RBCs

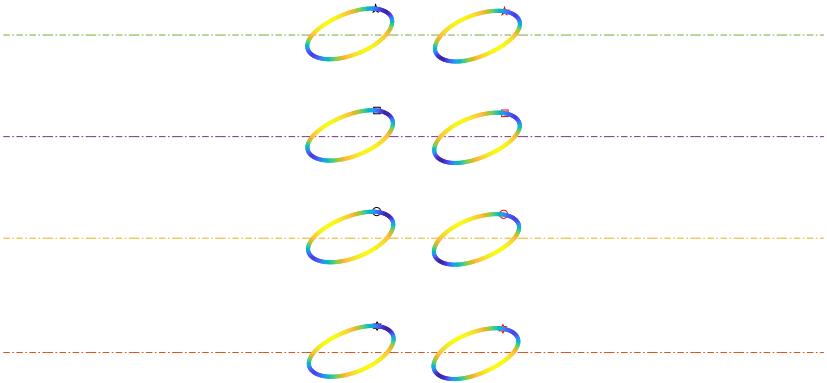


- Figure A: Healthy patient
- Figure B: Recent cardiac bypass patient
- Aggregate structure affects the blood rheology and viscoelasticity

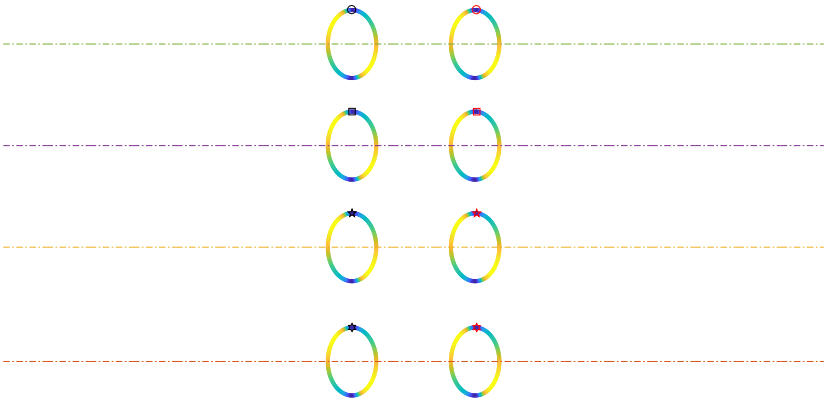
Reduced Area = 0.99



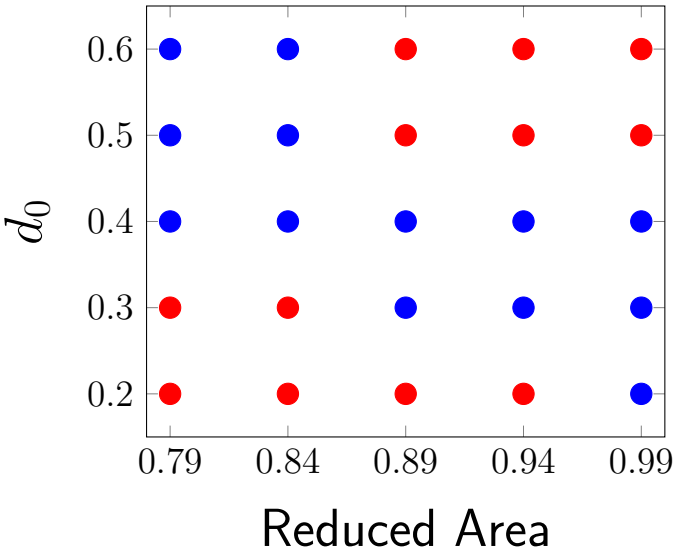
Reduced Area = 0.89



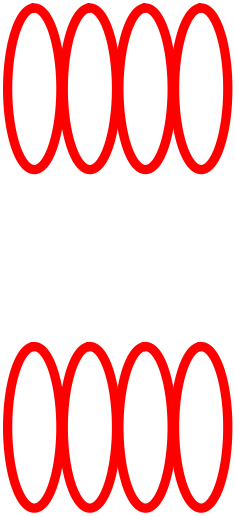
Reduced Area = 0.79



Formation of Doublets



Multiple Vesicles



Concluding Remarks

- Proposed an adhesion model based on a Lennard-Jones 4-2 potential
- Reliable high-fidelity solutions formed with high-order adaptive time stepping and near-singular integration
- The reduced area affects the nature of the near contact
- Doublets are formed with
  - Large reduced areas and small adhesion length scales
  - Small reduced areas and larger adhesion length scales