High-Order Adaptive Time Stepping of Vesicle Suspensions

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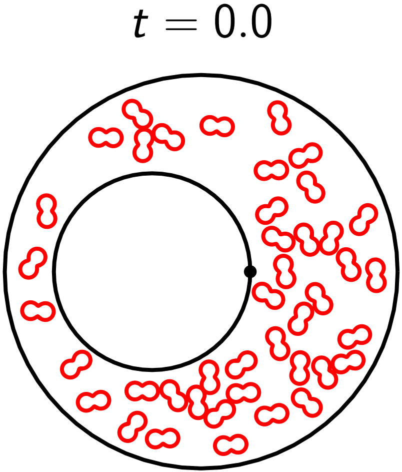
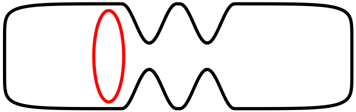
Outline

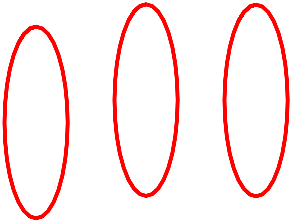
- Vesicle suspensions
- Numerical methods and algorithmic challenges
- High-order adaptive time stepping
- Low resolution simulations
- Concluding remarks



What is a vesicle?

- Deformable (2D) capsule filled and submerged in viscous fluid
- Boundary is locally inextensible
- Dynamics governed by hydrodynamic interactions with other vesicles/walls, resistance to bending and inextensibility
- Basic model for biomembranes such as red blood cells and platelets





Governing equations

Spectral representation

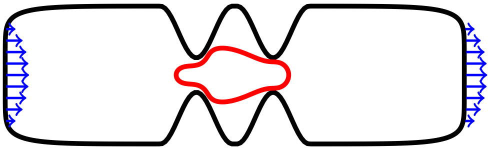
$$\mathbf{x}(\theta,t) = \sum_n \hat{\mathbf{x}}_n(t)e^{in\theta}$$

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

Fourier differentiation

$$\sigma_s = \frac{\sum_n in\hat{\sigma}_n(t)e^{in\theta}}{\left|\sum_n in\hat{\mathbf{x}}_n(t)e^{in\theta}\right|}$$

- Similar non-linear expression for $\mathbf{x}_{ssss}$



Vesicle equations

$$\frac{d\mathbf{x}}{dt} = \mathbf{v}_\infty + \mathcal{S}[\boldsymbol{\xi}] \qquad \mathbf{x} \in \gamma$$

$$0 = \text{div}_\gamma(\mathbf{v}_\infty + \mathcal{S}[\boldsymbol{\xi}]) \qquad \mathbf{x} \in \gamma$$

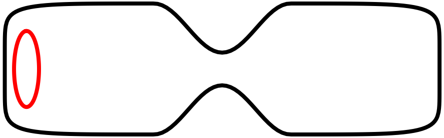
$$\boldsymbol{\xi} = \boldsymbol{\xi}(\mathbf{x},\sigma) = -\mathbf{x}_{ssss} + (\sigma\mathbf{x}_s)_s$$

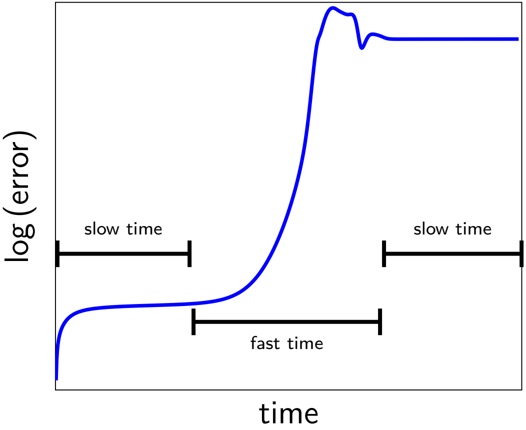
Stokes single-layer potential

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

Algorithmic challenges

- Moving boundaries
- High-order derivatives
- Stiffness
- Nearly touching interfaces
- Fast summations
- **High-order time adaptivity**
- Stability at low resolutions





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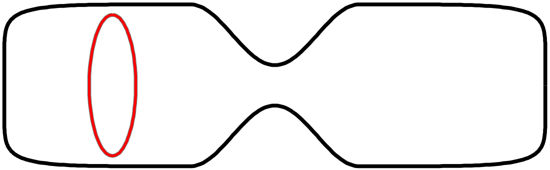
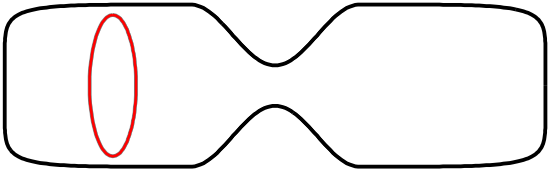




Semi-implicit time stepping

Quaife and Biros, J. Comput. Phys. 2014

Semi-implicit discretization is

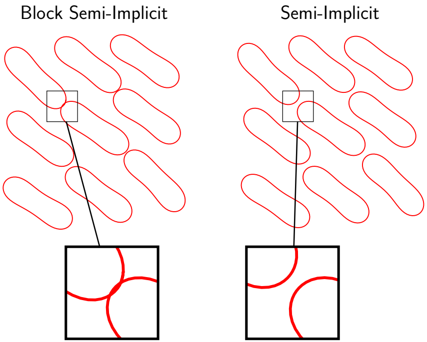
$$\frac{\mathbf{x}_j^{N+1} - \mathbf{x}_j^{N}}{\Delta t} = \mathbf{v}(\mathbf{x}_j^{N}; \mathbf{x}_j^{N+1}) + \sum_{k \neq j} \mathbf{v}(\mathbf{x}_j^{N}; \mathbf{x}_k^{N+1})$$

- Resolves self-interaction stiffness

$$\mathbf{x}_{ssss} \qquad \Delta t \sim N^{-3}$$

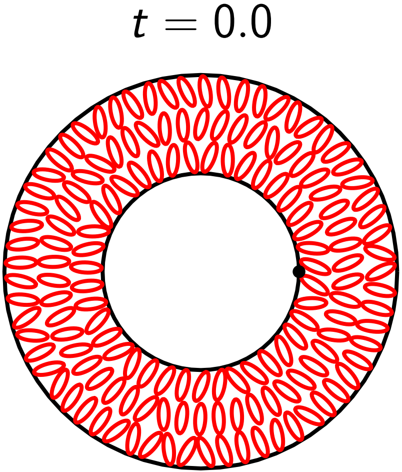
$$(\sigma \mathbf{x}_s)_s \qquad \Delta t \sim N^{-1}$$

- Resolves stiffness from nearly touching vesicles



Couette

- $N = 96$
- $N_{\text{wall}} = 256$
- $e_A = 7.3\text{E}{-3}$
- $e_L = 1.6\text{E}{-2}$
- 40.5 % volume fraction



Spectral deferred correction for vesicle suspensions

- Vesicle suspension governed by $\dot{\mathbf{x}}(t) = \mathcal{M}[\mathbf{x}](\mathbf{x})$
- Time stepping matrix is $\mathcal{M} = (\alpha I - \mathcal{D})^{-1}\mathcal{S}\mathcal{B}$
- Form provisional solution $\tilde{\mathbf{x}}$ of

$$\mathbf{x}(t) = \mathbf{x}_0 + \int_0^t \mathcal{M}[\mathbf{x}](\mathbf{x})d\tau$$

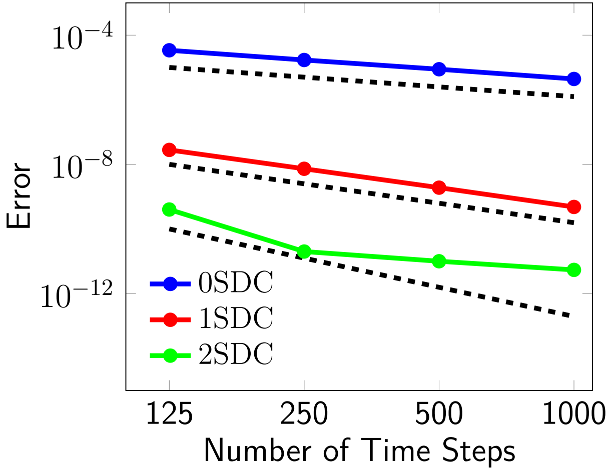
- Compute the residual

$$\mathbf{r}(t) = \mathbf{x}_0 - \tilde{\mathbf{x}}(t) + \int_0^t \mathcal{M}[\tilde{\mathbf{x}}](\tilde{\mathbf{x}})d\tau$$

- Define the new provisional solution $\tilde{\mathbf{x}} + \tilde{\boldsymbol{\delta}}$ where $\tilde{\boldsymbol{\delta}}$ approximates

$$\boldsymbol{\delta}(t) = \mathbf{r}(t) + \int_0^t (\mathcal{M}[\tilde{\mathbf{x}} + \boldsymbol{\delta}] - \mathcal{M}[\tilde{\mathbf{x}}])(\tilde{\mathbf{x}})d\tau + \int_0^t \mathcal{M}[\tilde{\mathbf{x}} + \boldsymbol{\delta}](\boldsymbol{\delta})d\tau$$

SDC convergence



- Gauss-Lobatto substeps used to compute residual
- Spatial errors, ill-conditioning, and GMRES tolerance restrict high-order convergence
- Order reduction

Adaptive time stepping

Quaife and Biros, J. Comput. Phys. 2016

- Automatically adjust Δt
- Crucial for problems with multiple time scales and long time horizons
- Error in area and length estimate the local truncation error

m	e_P	e_A	e_L
125	1.1E-4	3.4E-6	3.4E-5
250	5.3E-5	1.7E-6	1.7E-5
500	2.7E-5	8.8E-7	8.8E-6
1000	1.3E-5	4.4E-7	4.4E-6
125	1.4E-7	2.8E-8	1.3E-8
250	3.4E-8	7.3E-9	2.6E-9
500	8.3E-9	1.9E-9	4.5E-10
1000	2.0E-9	4.8E-10	6.9E-11

Time step size selection

- Solution accepted if $|A(t+\Delta t) - A(t)| \leq \epsilon A(t)\Delta t$
- Optimal time step size

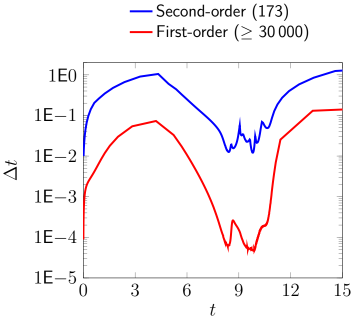
$$\Delta t_{\text{opt}} = \left(\frac{\epsilon A(t)\Delta t}{|A(t+\Delta t) - A(t)|}\right)^{1/k} \Delta t$$

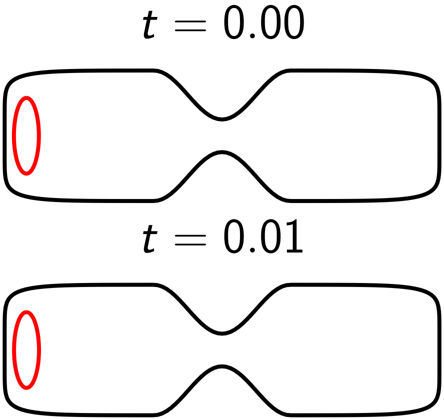
- New time step size

$$\Delta t_{\text{new}} = \alpha^{1/k} \min(\beta_{\text{up}}\Delta t, \max(\Delta t_{\text{opt}}, \beta_{\text{down}}\Delta t))$$

- $\alpha < 1$, $\beta_{\text{up}} > 1$, $\beta_{\text{down}} < 1$ are safety parameters

First- vs. second-order adaptive time stepping





- Much larger allowable time steps by using one SDC iteration
- 23X speedup for three digits of accuracy

Controlling the error

First-order: 0 SDC

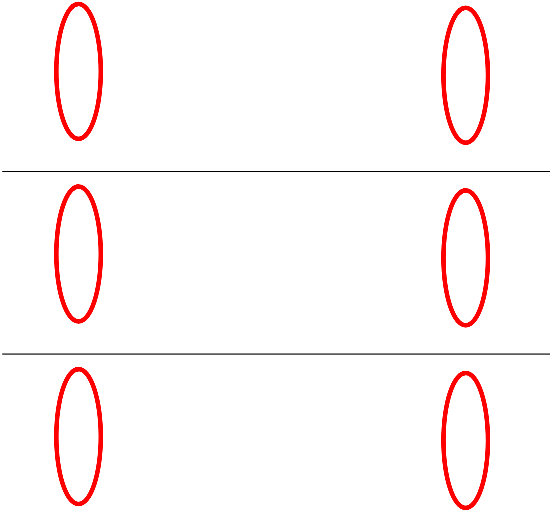
Tolerance	Error	Accepts	Rejects	$\mathcal{S}$ evals	CPU
1E−2	7.9E−3	3397	21	1.1E5	5.7
1E−3	9.4E−4	33554	12	1.1E6	59

Second-order: 1 SDC

Tolerance	Error	Accepts	Rejects	$\mathcal{S}$ evals	CPU
1E−2	2.6E−3	68	30	2.1E4	1.2
1E−3	5.6E−4	172	68	4.8E4	2.6

Tank treading and tumbling

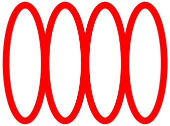
Quaife and Biros, Procedia IUTAM 2014

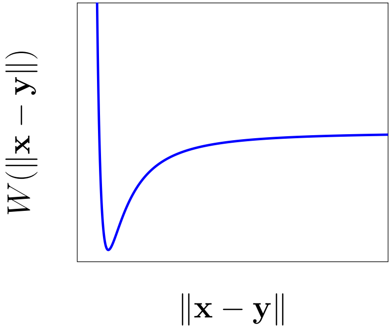


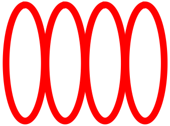
- Tank treading for $\nu < \nu_c$ and tumbling for $\nu > \nu_c$, $\nu_c \approx 4.05$
- 1 SDC correction
- Tolerance of 10^{-2}

Adding adhesion

$$\mathcal{W}(\mathbf{x}) := \sum_{k \neq j} \int_{\gamma_k} W(\|\mathbf{x} - \mathbf{y}\|) ds$$







Adaptive time stepping at low resolutions

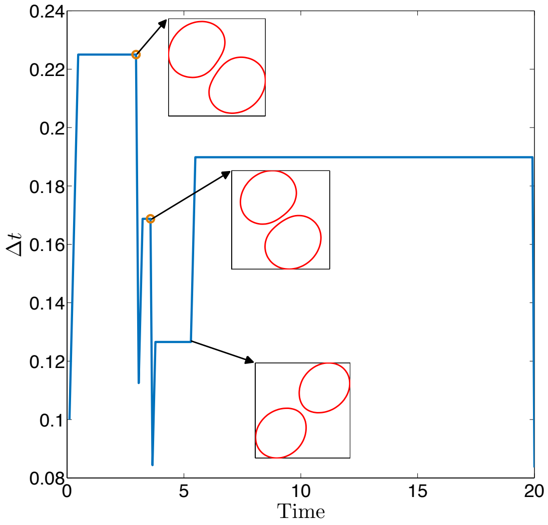
- Asymptotic estimates are invalid at low resolutions and large time step sizes
- If asymptotic estimates are invalid, change time step size by a constant factor

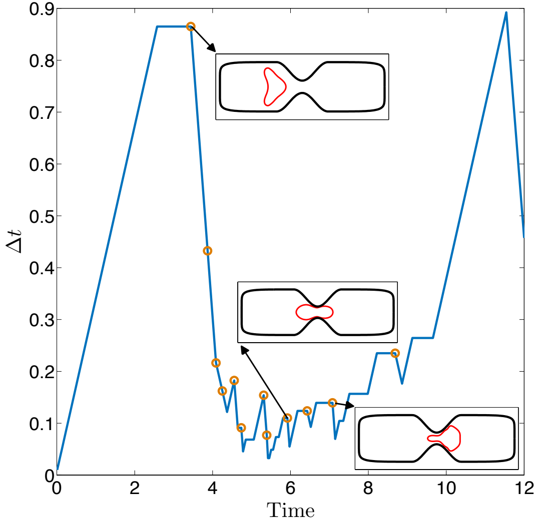
Time step selection

$A_{n+1} \leftarrow \texttt{getArea}(\mathbf{x}_{n+1})$ *compute area of new shape*
$q_A \leftarrow \texttt{computeTimeDerivaties}(\mathbf{x}_{n+1})$ *compute* $q_A = \left|\frac{dA}{dt}/A\right|$ *analytically*
$\epsilon_A \leftarrow \texttt{computeError}(A_{n+1}, A_n)$ *compute error in area*
if $\rho_{\min} \le \epsilon_A \le \rho_{\mathrm{AL}}$ **then** *error is marginally below tolerance*
    $\texttt{accept} = \texttt{true}$
    $\Delta t_{\mathrm{new}} = \Delta t_n$ *keep same time step size*
else if $\epsilon_A < \rho_{\min}$ **then** *error is substantially below tolerance*
    $\texttt{accept} = \texttt{true}$
    if $|\epsilon_A - q_A \Delta t| \le \rho_{\mathrm{up}} \epsilon_A$ **then** *asymptotic assumption is valid*
        $\Delta t_{\mathrm{new}} = \rho_{\mathrm{AL}}/q_A$
    else *asymptotic assumption is invalid*
        $\Delta t_{\mathrm{new}} = \beta_{\mathrm{up}} \Delta t_n$
    end if
else if $\epsilon_A > \rho_{\mathrm{AL}}$ **then** *error is greater than tolerance*
    $\texttt{accept} = \texttt{false}$
    if $|\epsilon_A - q_A \Delta t_n| \le \rho_{\mathrm{down}} \epsilon_A$ **then** *asymptotic assumption is valid*
        $\Delta t_{\mathrm{new}} = \rho_{\mathrm{AL}}/q_A$
    else *asymptotic assumption is not valid*
        $\Delta t_{\mathrm{new}} = \beta_{\mathrm{down}} \Delta t_n$
    end if
end if
return $\Delta t_{\mathrm{new}}, \texttt{accept}$

Adaptive time stepping at low resolutions

Kabacaoglu, Quaife, and Biros, J. Comput. Phys. 2018





Summary

Conclusions

- High-order adaptivity achieved with IMEX Euler and SDC
- Used error in area and length to estimate local truncation error
- No trial and error procedure to find correct time step size

Future Work

- Better understanding of order reduction for SDC
- Multirate time integrator
- Parallel implementation