High-order adaptive time stepping for deformable capsules

Bryan Quaife and George Biros
Department of Scientific Computing, Florida State University

Abstract
An adaptive high-order time-stepping scheme for the flow of vesicles suspended in a Stokesian fluid is developed. A spectral deferred correction (SDC) method is used to iteratively increase the order of a first-order implicit-explicit (IMEX) time integrator. For adaptive time stepping, invariant properties of vesicles, constant area and length, are used to reduce the computational cost. We demonstrate that the proposed scheme enables automatic selection of the time step size and high-order accuracy.

Introduction
Vesicles are deformable capsules that are:
• Submerged in an incompressible Stokes flow
• Resist bending
• Locally inextensible
• Used to model capillary blood flow
Fluid and vesicle equations are
\[ \frac{\Delta u}{\Delta t} = \mathbf{f}(x, u), \quad \nabla \cdot u = 0, \quad u \in \Omega \]
\[ \Delta \frac{\partial u}{\partial t} = \mathbf{f}(x, u), \quad \nabla \cdot u = 0, \quad u \in \gamma \]
Boundary integral equation formulation places all unknowns on vesicle interface
\[ \frac{\partial u}{\partial n} - \int_{\Gamma} S^T(x, y) \sigma(y) dy \]
Stokesian boundary conditions:
• Confinement requires an additional double-layer potential on the solid wall
• Viscosity contrast requires an additional double-layer potential on the vesicle interface
• Other physics such as adhesion, surfactants, and electric potentials can be added

Spectral deferred correction
• Largely based on [3] and [6]
• First-order provisional solution \( \langle k, \lambda \rangle \) at \( 0 = \tau_0 < \cdots < \tau_p = \tau \) formed with IMEX scheme
\[ x^{n+1} = x^n + \Delta \tau_\lambda x^{n+1} \left[ \int x^T x^{n+1} + T x^{n+1} \right] \]
• Quadrature approximates residual \( r \)
• Error satisfies
\[ e_{\text{err}}(\tau) = \varepsilon(x, y) + \int_{\partial \Omega} \left[ S(x, y) T(x, y) \right] \sigma(y) dy \]
• First-order solution of \( e_{\text{err}}(\tau) \) formed with
\[ x^{n+1} = x^n + \Delta \tau_\lambda x^{n+1} \left[ \int x^T x^{n+1} + T x^{n+1} \right] \]
• Update \( x = x + \Delta \tau_\lambda x^{n+1} \) and iterate

Adaptivity
• Error in area and length estimate the local truncation error \( E(\tau) \)
• If tolerance is \( \epsilon \), time step accepted if
\[ |E(\tau + \Delta \tau) - E(\tau)| < \epsilon |E(\tau)\Delta \tau| \]
• For order \( k \) method, new optimal time step size is
\[ \Delta \tau_k = \left( \frac{E(\tau + \Delta \tau) - E(\tau)}{|E(\tau)\Delta \tau|} \right)^{1/2} \]
• Safety parameters restrict how quickly the time step size changes

Numerical examples
• Poiseuille flow at intake and outtake
• Extra digit of accuracy achieved for comparable cpu times
• 1 cpu time is 1 hour

Stenosis:
• Single vesicle in a relaxation flow
• Speculate that each SDC iteration gives an extra order of accuracy
• Bending results in ill-conditioning (no more than 10 digits accuracy)
• Techniques to reduce order reduction are under consideration [4]

Turbulent flow:
• Shear flow
• Vesicles with viscosity contrast greater than 4.2 tumble, otherwise they tank tread
• Desired error is 1E-2 and final error is 9.96E-3

Couette:
• Inner boundary rotating with constant angular velocity
• Avoid trial-and-error procedure to find acceptable time step size
• 1 cpu time is 3.5 days

Discussion
• Developed a spectral deferred correction (SDC) algorithm for vesicle suspensions
• Time integrator is self starting and compatible with adaptive time step sizes
• Local truncation error efficiently estimated with error in length and area
• Order reduction needs to be analyzed and removed [4]
• Can be applied to other deformable capsules such as bubbles, polymers, and foams
• Considering a multirate time integrator

References