Review of *Adaptive Time Stepping for Vesicle Suspensions*

Some general comments: This paper has two main contributions. First a non-standard SDC method is introduced for the integral-differential equations governing vesicle suspensions. The advantage of this approach is that presumably it allows for the construction of higher-order accurate self starting temporal methods. Secondly, a procedure for adjusting the time step based on the error in two invariants in 2-D vesicle flow is tested. In my opinion the paper will be of interest to a diverse audience, and the ideas are significant enough to merit publication. I do however have two main objections to the paper which I think need to be cleared up before it can be published.

Objection 1. I think the presentation in this paper generates some confusion on the issue of the accuracy of SDC in the stiff regime. The paper does report on the early results on order reduction (e.g. [26]), but the issue is much better understood now than when [26] was written. In [18] for example, the authors show that the order-reduction previously observed for SDC for stiff problems is equivalent to the slow convergence of the numerical solution to that given by a fully implicit Gaussian collocation scheme (or equivalently a fully implicit Gauss-Runge-Kutta method). This subtle shift from viewing SDC as a method using a fixed number of iterations to achieve a fixed order of accuracy to viewing SDC as an iterative procedure that converges to a spectrally accurate collocation method is really the key to understanding the behavior for stiff problems.

Although Thms like the 2.1 cited here show that the formal order of accuracy of SDC increases in lock-step with the number of correction iterations, these results are only observed asymptotically as the time step approaches zero. For stiff problems, the iterations for explicit SDC methods will diverge in k for sufficiently large time step. For fully implicit methods the convergence of SDC iterations in k will slow down, and order reduction is observed. Hence there are two "convergences" going on: the convergence in iteration k where the SDC solution approaches the collocations solution and the convergence in Δt as the numerical solution approaches the exact solution. The citation [44] examines the first convergence carefully for linear problems. If the simulations are always done with enough SDC iterations so that the iterations have converged in k (or some sort of acceleration of the convergence is used), then the observed convergence rate will be that of the collocation scheme (which is not necessarily the order in the non-stiff case. See for example Hairer and Wanner II). If a fixed number of iterations are used, the asymptotic rate may not be observed until Δt is sufficiently small, i.e. order reduction is seen.

Unfortunately, the numerical results presented here mix these issues up. For the test in 5.1, p=5 nodes are used, so that if many SDC iterations are used, the observed rate should be 8. For a fixed number of iterations, order k convergence should be observed for sufficiently small Δt, but this is obscured because of machine precision (and GMRES precision). It is not really clear why one would choose p=5 nodes and 2, 3 or 4 iterations anyway due to the fact that it requires more storage for the same order of accuracy as using fewer nodes. Similar issues are appropriate for other tests.

So in summary, the use SDC methods for stiff problems leads to a very subtle trade off. Using enough iterations so that the SDC iterations converge (which can be checked by monitoring the residual) requires more work, but insures the optimal order of accuracy and

stability of the Gauss collocation schemes. Using a fewer fixed number means that the order for stiff problems will be reduced. This paper proceeds with numerical convergence tests as if the problems are not stiff, and hence will add confusion to the question of order of accuracy.

Finally, the formulas like that for C_A appearing on page 11, directly use assume the order of the scheme. In the stiff limit, these are only valid when the SDC iterations have converged. So it would seem that a to use this sort of estimate for higher-order SDC, one would need to monitor the residual as well.

Objection 2. In my opinion, the use of only the length and area of the vesicles as a measure of error is a major short-coming in the numerical experiments, particularly in light of the results on the demonstrated order of accuracy. The SDC method is applied to the position of vesicle markers, hence the most appropriate measure of error would be a norm of the error in position at a fixed time. This of course has the disadvantage that the error would have to be approximated by comparison to a reference solution, but this is not reasonable grounds for exclusion of such results. Accurate computation of particle trajectories will imply that the vesicle length and area remain accurate, but the converse is not true. For simulations with many vesicles moving in complex flows, the exact position of each may not be the most relevant finding, but in terms of demonstrating the accuracy and order of convergence of a new numerical approach, convergence of position error should be demonstrated.

A related issue: How are the length and area of the vesicles actually computed? Is it the case that these are spectrally accurate as well?

Specific comments: This paper could be improved substantially by more careful writing. Some suggestions:

- pg 1. The first sentence of the abstract mentions an "arbitrary-order accurate" method. Given the ambiguous evidence of even 3rd order accuracy in time, I think this characterization is inappropriate.

- pg. 2 first paragraph. ,"implicit higher-order meth- ods are quite challenging to combine with adaptive schemes. The most common methods are implicit multistep schemes, but those are problematic especially for dynamics that involve moving interfaces." I am not sure here what the authors mean. Combining multistep methods with adaptive time stepping does require more work than single step methods, but that holds true for both implicit and explicit. Why do moving interfaces make the things "especially problematic"?

- pg 2 second paragraph. You might explain why a standard stiff DIRK method does not meet you design goals.

- pg 2, "The incompressibility and inextensibility conditions require that the vesicle preserves both its enclosed area and total length." You should be clear that this is true only in two dimensions.

- pg 2., "These are relatively easy to implement but inefficient due to bending stiffness." It is not the bending stiffness, but rather the small time step that the bending stiffness necessitates.

- pg 2, "grouped in three classes of methods" There are no citations given for the first two classes. Do they actually exist?

- pg 2, and beyond: "a first order backward Euler scheme" "first order" should be hyphenated when used as an adjective.

- pg 4. "Any time stepping scheme can be used to generate a provisional solution". Time stepping schemes do not produce a continuous function of t. This explanation of SDC mixes up approximate continuous solutions and approximate discrete solutions. The former can be constructed from the latter by standard interpolation. The notation needs to cleared up here to differentiate between discrete and continuous approximate solutions.

- pg. 5, the equation for vesicle suspensions contain a confusion mix of $\mathbf{x_k}, \mathbf{x}, \mathbf{y}, \mathbf{x}'$.

- pg. 7. This section at the top of the page would be much clearer if it was described on a timestep $[t_n, t_{n+1}]$. This is almost done in the first line of the page, but below the integrals always say $t \in [0, T]$, which is misleading at best.

- pg 10 paragraph starting "A common strategy of an adaptive time step method is to control an estimate of the local truncation error. One estimate is the difference of two numerical solutions". Some specific citations are appropriate here.

- pg 11 "it is dangerous to change the time step size ..." What is the danger?

- pg 13 first paragraph in 5.1, the maximum accuracy using 5 Lobatto nodes is 8, not seven.

- Table 1 and beyond: These tables are tedious. Log plots of errors make understanding convergence so much easier.

- Table 5-9. There is too much content in the captions of these tables. Some is redundant and should be omitted while some should be moved to the discussion.

- pg 18, first bullet. It makes no sense that 6,000 fixed time steps gives the same number of digits as 30,000 adaptive time steps. Is this a typo?

- Figure 6. Again, the caption is very long.

- pg 23, last bullet. In 3d, the use of length and area become volume and surface area. Are these quantities readily computable with the accuracy necessary to choose the time step?

- pg 24-25 the SDC sweeps described here look like procedures for stepping from $[t_n, t_{n+1}]$ where typically SDC is described by sub-stepping between quadrature nodes in $[t_n, t_{n+1}]$ (often denoted t_m). Also, one of the novel things about this method is the mixing of terms both implicit and explicit and from SDC iteration k and $k+1$ (or here tilde and not tilde). This should be emphasized in the description.