

An Eulerian-Lagrangian method for simulating the interaction of a Non-Newtonian fluid with complex shaped micro-swimmers

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I Method

The numerical method used for the Eulerian part of our micro-swimmer simulations is a staggered grid, dynamic adaptive mesh refinement algorithm for incompressible multi-phase flow. The dynamics of the micro-swimmer geometry, represented on a Lagrangian grid, is coupled to the Eulerian fluid flow by way of converting the Lagrangian representation of the micro-swimmer to a Moment-of-Fluid Eulerian representation. The details of the numerical method, excluding the staggered grid treatment for the non-Newtonian force terms, are presented in the following journal articles: [1, 3, 5, 6].

It is important to note that our results presented here correspond to a staggered grid formulation which is known to have better stability properties than the collocated formulation [9]. The source of the stability problems for a collocated grid algorithm is that the pressure projection step corresponding to the collocated formulation has a non-empty null space in the pattern of a checkerboard velocity distribution.

The numerical algorithm for simulating non-Newtonian multi-fluid/multi-phase flows that was presented in [5] was for a collocated grid. The numerical algorithm presented in [6] was for a staggered grid, but only Newtonian flows were simulated in [6]. The non-Newtonian multi-fluid/multi-phase results presented in this report are distinct from [5] in that the present results were computed on a staggered grid.

The potential pitfalls of the collocated formulation notwithstanding, in Figures 1, 2, and 3 below, it is observed that the collocated results of the past agree, qualitatively, with the present staggered grid results. This is encouraging, since the present results (a) reinforce that the previous reported collocated results were “reasonably valid” and did not suffer from stability problems, and (b) reinforce that the present staggered grid method has been implemented “reasonably correctly,” and has a mathematical guarantee of stability [4] for future simulations.

The mathematical model governing our numerical method is given as follows:

$$\nabla \cdot \vec{u} = 0 \quad (1)$$

$$\frac{\partial(\rho\vec{u})}{\partial t} + \nabla \cdot (\rho\vec{u}\vec{u}^T) = \nabla \cdot (-p\mathbf{I} + \boldsymbol{\tau}) \quad (2)$$

$$\boldsymbol{\tau} = \boldsymbol{\tau}_s + \boldsymbol{\tau}_p \quad (3)$$

$$\boldsymbol{\tau}_s = 2\mu_s \mathbf{D} = \mu_s(\nabla\vec{u} + \nabla\vec{u}^T) \quad (4)$$

$$\boldsymbol{\tau}_p = \frac{\mu_p \mathbf{f}^s(\mathbf{A})}{\lambda} \quad (5)$$

$$\overset{\nabla}{\mathbf{A}} \equiv \frac{\partial \mathbf{A}}{\partial t} + \nabla \cdot (\vec{u}\mathbf{A}) - \mathbf{A} \cdot \nabla\vec{u} - (\nabla\vec{u})^T \cdot \mathbf{A} = -\frac{f_R(\mathbf{A})}{\lambda} \quad (6)$$

$$\frac{\partial\phi_m}{\partial t} + \vec{u} \cdot \nabla\phi_m = 0 \quad m = 1, \dots, M \quad (7)$$

\vec{u} is the fluid velocity, ρ is the density which can have large jumps at material interfaces, p is the pressure, and $\boldsymbol{\tau}$ is a combination of the solvent stress tensor $\boldsymbol{\tau}_s$ and polymer stress tensor, $\boldsymbol{\tau}_p$. μ_s is the solvent viscosity

which can have large jumps at material interfaces, \mathbf{D} is the rate of deformation tensor, $bmD = \nabla \vec{u} + \nabla \vec{u}^T$, and \mathbf{A} is the configuration tensor. ϕ_m is the level set function for material m ($m = 1, \dots, M$) and satisfies,

$$\phi_m(t, \vec{x}) = \begin{cases} +d_m & \text{if } \vec{x} \text{ is in material } m \text{ at time } t \\ -d_m & \text{if } \vec{x} \text{ is not in material } m \text{ at time } t. \end{cases} \quad (8)$$

d_m in (8) represents the closest distance from point \vec{x} to the material m interface. The relaxation source term $f_R(\mathbf{A})$ found in (6) is defined as follows

$$f_R(\mathbf{A}) = \begin{cases} \frac{\mathbf{A}}{1-\text{tr}(\mathbf{A})/L^2} - \mathbf{I} & \text{FENE-P model} \\ \frac{\mathbf{A}-\mathbf{I}}{1-\text{tr}(\mathbf{A})/L^2} & \text{FENE-CR model} \end{cases} \quad (9)$$

The polymer stress versus strain term $f_s(\mathbf{A})$ found in (5) is defined as follows

$$f_s(\mathbf{A}) = \begin{cases} \frac{\mathbf{A}}{1-\text{tr}(\mathbf{A})/L^2} - \mathbf{I} & \text{FENE-P model} \\ \frac{\mathbf{A}-\mathbf{I}}{1-\text{tr}(\mathbf{A})/L^2} & \text{FENE-CR model} \end{cases} \quad (10)$$

We refer the reader to the following references for more information on the mathematical models for non-Newtonian fluids [2, 8].

The (novel) results presented in this report are preliminary in that we only present results for the one-way coupling between the swimmer (prescribed Lagrangian description of its motion) and the non-Newtonian fluid (Eulerian description of its motion). The prescribed swimmer motion influences the fluid motion but the fluid motion does not in turn effect the swimmer motion. The swimmer (see Figures 2 and 3) undergoes rigid body motion in the form of translation along the z axis, $\vec{u}_{translate} = (0, 0, w)$ and rotation about the z axis $\vec{u}_{rotate} = (-\Omega y, \Omega x, 0)$:

$$\frac{d\vec{x}_{swimmer}}{dt} = \vec{u}_{translate} + \vec{u}_{rotate}. \quad (11)$$

The Eulerian fluid motion is coupled to the prescribed Lagrangian swimmer motion by way of the no-slip condition,

$$\vec{u}_{fluid}(t, \vec{x}) = \vec{u}_{translate}(\vec{x}) + \vec{u}_{rotate}, \quad (12)$$

which is satisfied by all points \vec{x} on the swimmer surface at time t .

II Results

Two types of results are presented in this report: (A) verification results, and (B) validation results.

II.1 Verification Results: Rising gas bubble in non-Newtonian fluid

In Figure 1 we compare computational results for the rise of a gas bubble in a hybrid shear thinning and FENE-CR liquid solution [5]. The model parameters for this test correspond to the parameters used in [5] (see Figure 7 from [5]). The viscoelastic model is the hybrid Shear thinning Carreau and FENE-CR model. The specific non-Newtonian model parameters are $n = 1/2$, $L = 10$, and $De = 5$. We expect to compute a bubble that attains a very unique “cusped-cap” shape.

In our Figure 1, we show the following 3 results: (a) collocated results from [5], (b) staggered quarter domain 3D results (mirrored across the $x-z$ and $y-z$ planes for comparison purposes) computed using

our latest algorithm, and (c) staggered 3D RZ (axisymmetric R - Z) results (revolved about the z axis for comparison purposes).

With the latest staggered grid method, we are able to reproduce the cusped cap shape that was computed with a collocated grid method. We remark that our new results are not in quantitative agreement with the previous collocated results, this can be attributed to either (a) not having enough data to compare at precisely the same simulation time, or (b) a difference in treatment of the interface jump conditions where a Newtonian gas meets with a Non-Newtonian liquid.

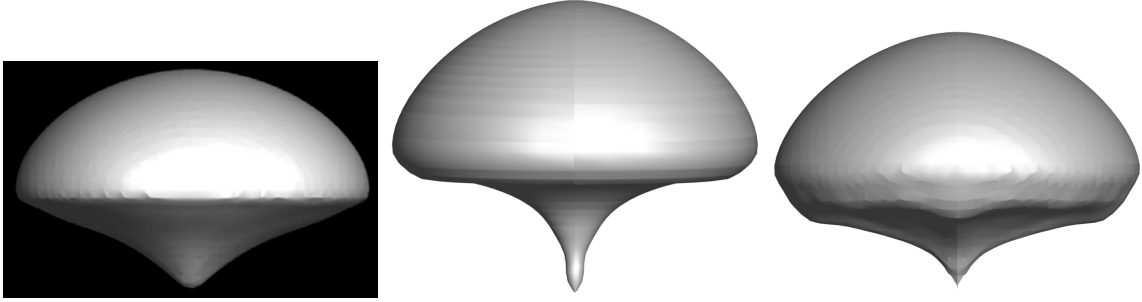


Figure 1: Comparison between staggered and non-staggered algorithms for a gas bubble rising in a non-Newtonian fluid; from left to right: (a) collocated results 3D, (b) staggered results, 3D axis-symmetric, at time $t = 0.434$, (c) staggered results, 3D, quarter domain simulation at time $t = 0.472$.

II.2 Validation Results and Discussion: Helical swimmer in non-Newtonian fluid

In Figures 2 and 3 we compare previous results for the Q_{11} component of the configuration tensor using the collocated algorithm with the current staggered grid algorithm. The pitch angle in Figure 2 is 12.4 degrees and the pitch angle in Figure 3 is 47.5 degrees. The liquid surrounding the swimmer is modeled as a FENE-P fluid. The rotational velocity of the Helical swimmer for all of the simulations reported here is $\Omega = 2\pi$ radians per second. The translational motion for both staggered grid simulations was 0.00355 cm/s. Unfortunately, after the simulations were completed, it was discovered that the translational motion for the 12.4 degrees collocated case was 0.015 cm/s and the translational motion for the 47.5 degrees collocated case was 0.027 cm/s.

As is shown in the two comparison Figures, 2 and 3, we have qualitative agreement between the previous collocated algorithm and the present staggered grid algorithm. Whereas the distribution of Q_{11} is in agreement, there is disagreement in the magnitude of Q_{11} . We attribute this disagreement to the following: (a) the translational velocity was different between the collocated simulations and the staggered grid simulations, (b) the treatment of the boundary conditions where the non-Newtonian liquid interacts with the dynamic helical swimmer is different between the two formulations, and (c) (perhaps the biggest reason for the difference) the recent staggered grid swimmer results implemented more aggressive adaptive mesh refinement which has the benefit of more efficient use of available computer resources, but at the cost of less accuracy on the coarse parts of the computational domain.

III Conclusions

A new staggered grid numerical method has been developed for simulating the Eulerian-Lagrangian interaction of a “Helical Micro-swimmer” with the surrounding Non-Newtonian fluid. In comparing the present (novel) staggered grid numerical method for non-Newtonian multi-phase, multi-fluid flow with the previous

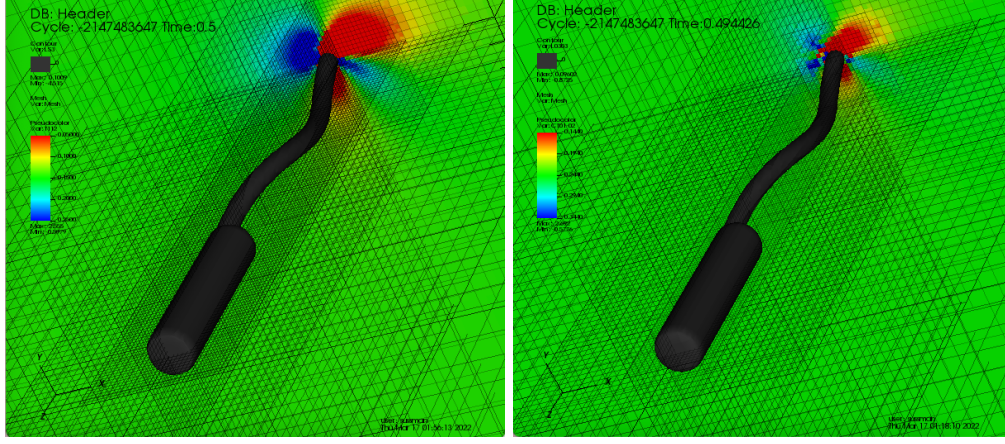


Figure 2: Comparison (Q_{11} component) between staggered and non-staggered algorithms for non-Newtonian FENE-P flow past a helical swimmer with pitch angle $12p$ degrees. (a) left: collocated results, (b) right: staggered results, at time $t = 0.5$.

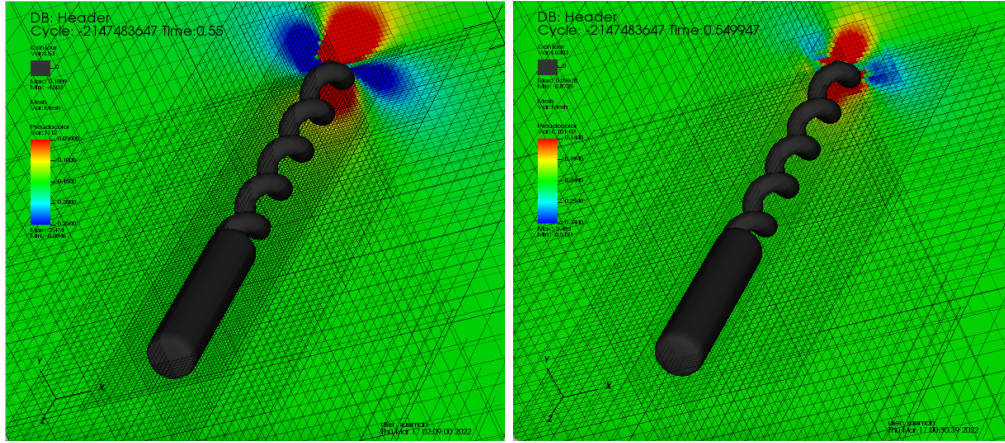


Figure 3: Comparison (Q_{11} component) between staggered and non-staggered algorithms for non-Newtonian FENE-P flow past a helical swimmer with pitch angle 47.5 degrees. (a) left: collocated results, (b) right: staggered results, at time $t = 0.55$.

collocated grid results, we have observed qualitative agreement. In the results section above, we report on our reasonings for the lack of quantitative agreement. We believe the quantitative differences can be resolved in the future. The staggered grid method is beneficial, all things considered, because the method has inherent stability properties [4] which will become important in the future when simulating Eulerian-Lagrangian interaction phenomena with more energetic forcing terms. Also it is planned for the future to include fluctuating hydrodynamics modeling [7, 10] into our simulations.

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