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Efficient numerical techniques for modelling of surfactant-laden interfacial phenomena

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Numerical scheme. We developed a direction-splitting scheme that allows to integrate the incompressible Navier-Stokes equations and the equations for the bulk and surface concentration of a surfactant γ:

$$\begin{cases} \rho\left(\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u}\right) + \nabla p - \nabla\cdot\left(\mu(\nabla\boldsymbol{u} + \nabla\boldsymbol{u}^T)\right) = f \ in\ \Omega\times[0,T] \\ \nabla\cdot\boldsymbol{u} = 0 \qquad in\ \Omega\times[0,T] \\ \boldsymbol{u} = \boldsymbol{0}, \quad in\ \partial\Omega\times[0,T], \quad \boldsymbol{u}|_{t=0} = \boldsymbol{u_0}, \quad in\ \Omega. \end{cases}$$

$$\frac{\partial\gamma}{\partial t} + \nabla_s\cdot(\boldsymbol{u}_s\gamma) = D_s\nabla_s^2\gamma + j_s, \quad on\ \Gamma,$$
$$\frac{\partial(\delta_\Gamma\gamma)}{\partial t} + \nabla\cdot(\gamma\delta_\Gamma\boldsymbol{u}) = \nabla\cdot(\delta_\Gamma D_s\nabla\gamma) + \delta_\Gamma j_s, \quad in\ \Omega,$$

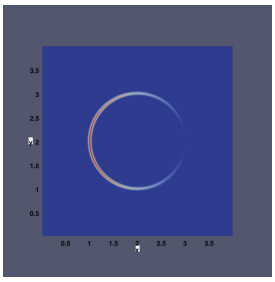
It integrates implicitly all equations requiring the solution of tri-diagonal subproblems only. This procedure allows also for an easy and scalable parallelization of the algorithm. For details, see [1], [2]. The method is implemented in a 2d and 3d parallel code using the MPI library. The code has been validated on a set of benchmark problems available in the literature.

Numerical Tests. Here we present just two of the verification examples. The complete procedure and the full set of numerical results will be published in an article that is currently in preparation.
Example 1. Consider a stationary circle with radius R and initial surface concentration

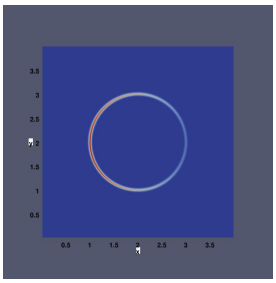
$$\gamma_0 = \frac{1}{2}(1-\cos(\theta)),$$

where θ is the angle measured in the counter clockwise direction from the y-axis. We run the code with $\epsilon = 4h$, where h is special step size, $\tau = 0.001$ and 200 interior points. This example shows the diffuse interface representation of the surface concentration equation. The results are shown in the following figure.

Figure 1



a) Fixed circle at time t=0

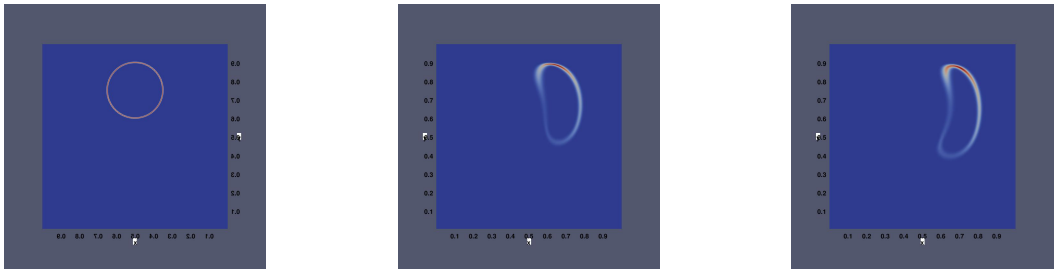


b) Fixed circle at time t=1

Example 2. Consider a circle with radius r=0.15 centered at $(0.5, 0.75)$ in domain $\Omega = [0,1]\times[0,1]$. The velocity field is $\begin{matrix} u = -\cos(\pi t)sin^2(\pi x)\sin(2\pi y), \\ v = \cos(\pi t)sin^2(\pi y)\sin(2\pi x). \end{matrix}$ The initial concentration is set to be $\gamma_0 = 10^{-4}$ and the initial bulk concentration is $C_0 = 10^{-4}y$ which is non-uniform. The adsorption and desorption coefficients are $r_a = 100$ and $r_d = 200$. We took the interface thickness $\epsilon = 4h$ with grad spacing

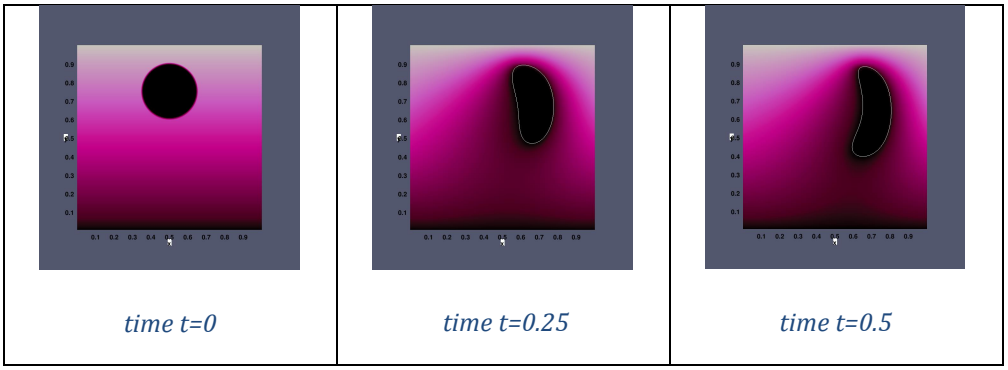
$h = 1/500$ and $D_s = 1.0$. The results for both surfactant and bulk concentration at three different times are shown in figures 2 and 3 correspondingly.

Figure 2



time t=0 *time t=0.25* *time t=0.5*

Figure 3



time t=0 *time t=0.25* *time t=0.5*

Impact on the career of the PI. The PI acquired a very efficient tool for simulation of interface problems with surfactants. It will be further used to study such problems at various regimes. The first one will be the problem for the dynamics of the liquid film entrained in the process of withdrawing a substrate from a fluid containing a surfactant. The new code allows for very high resolution simulations since it can be run on large clusters and therefore solve problems with billions of degrees of freedom.

Impact on the career of the postdoctoral fellow and students. Peyman Hessari has just started his career as a lecturer at the Grand Prairie College. The research experience acquired in the project helped him secure this job since this college is planning to grow into a university and hires teachers with clear research interests. We are completing the first paper from the project. He will continue to work in this direction further, and is planning to apply for an NSERC grant to support his research. The students involved in the code development acquired valuable skills on coding in a parallel environment and learned the basics of the discretization of problems with free boundaries and splitting methods.

[1] J.L. Guermond and P. Minev, High-order time stepping for the Navier-Stokes equations with minimal computational complexity. **J. Computational and Applied Mathematics**, 310 (2017), 92-103.

[2] P. Minev abd P. Vabishchevich, Splitting schemes for unsteady problems involving the grad-div operator. **Applied Numerical Mathematics**, 124 (2018), 130-139.