Semi-Implicit Scheme for low Mach Fluctuating Hydrodynamics

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We want to solve the low Mach equations for large Schmidt number, $\nu \gg \chi$, so that viscosity has to be handled implicitly. I propose a scheme where concentration is handled explicitly using a predictor-corrector framework and only viscosity is handled implicitly. I do not now how to do both implicitly in a doable manner. Since we are implicit in velocity here instead of using momentum we will only use velocity and therefore use the affine operator $\boldsymbol{\mathcal{P}}_S$ (rather than $\boldsymbol{\mathcal{P}}_F$), defined via its action on a vector field $\boldsymbol{w}$,

$$\boldsymbol{\mathcal{P}}_S(\boldsymbol{w}) = \boldsymbol{w} - \rho^{-1}\boldsymbol{\nabla}\left[\boldsymbol{L}_\rho^{-1}(\boldsymbol{\nabla}\cdot\boldsymbol{w} - S)\right]. \tag{1}$$

Recall that $S(\boldsymbol{F}) = -(\rho^{-1}\beta)\ \boldsymbol{\nabla}\cdot\boldsymbol{F}$ is a function of $\boldsymbol{F}$ and the same goes for $\boldsymbol{\mathcal{P}}_S$.

1 Predictor-Corrector Algorithm

1. Calculate predictor diffusive and stochastic fluxes,

$$\boldsymbol{F}^n = (\rho\chi\boldsymbol{\nabla}c)^n + \sqrt{\frac{2\left(\chi\rho\mu_c^{-1}\right)^n k_B T}{\Delta t\,\Delta V}}\,\widetilde{\boldsymbol{W}}^n,$$

   and then evaluate S^n from $\boldsymbol{F}^n$.

2. Take a predictor forward Euler step for ρ_1 and ρ,

$$\begin{aligned}\rho_1^{\star,n+1} &= \rho_1^n + \Delta t\,\boldsymbol{\nabla}\cdot\left(-\rho_1^n\boldsymbol{v}^n + \boldsymbol{F}^n\right)\\ \rho^{\star,n+1} &= \rho^n + \Delta t\,\boldsymbol{\nabla}\cdot\left(-\rho^n\boldsymbol{v}^n\right).\end{aligned}$$

3. Calculate corrector diffusive fluxes, and reuse the same random numbers,

$$\boldsymbol{F}^{\star,n+1} = (\rho\chi\boldsymbol{\nabla}c)^{\star,n+1} + \sqrt{\frac{2\left(\chi\rho\mu_c^{-1}\right)^{\star,n+1} k_B T}{\Delta t\,\Delta V}}\,\widetilde{\boldsymbol{W}}^n.$$

4. Take a predictor Crank-Nicolson step for the velocity by solving a Stokes system for $\boldsymbol{v}^{\star,n+1}$ and $\pi^{\star,n+1}$,

$$\begin{aligned}\frac{\rho^{\star,n+1}\boldsymbol{v}^{\star,n+1} - \rho^n\boldsymbol{v}^n}{\Delta t} + \boldsymbol{\nabla}\pi^{\star,n+1} &= \boldsymbol{\nabla}\cdot\left(-\rho^n\boldsymbol{v}^n\boldsymbol{v}^n\right) + \frac{1}{2}\left(\rho^n + \rho^{\star,n+1}\right)\boldsymbol{g}\\ &+ \frac{1}{2}\boldsymbol{\nabla}\cdot\left(\eta^n\bar{\boldsymbol{\nabla}}\boldsymbol{v}^n + \eta^{\star,n+1}\bar{\boldsymbol{\nabla}}\boldsymbol{v}^{\star,n+1}\right) + \boldsymbol{\nabla}\cdot\left[\sqrt{\frac{\eta^n k_B T}{\Delta t\,\Delta V}}\left(\boldsymbol{W}^n + (\boldsymbol{W}^n)^T\right)\right],\\ \boldsymbol{\nabla}\cdot\boldsymbol{v}^{\star,n+1} &= S^{\star,n+1},\end{aligned}$$

   where $\bar{\boldsymbol{\nabla}} = \boldsymbol{\nabla} + \boldsymbol{\nabla}^T$ denotes a symmetrized gradient.

5. Update the densities and concentrations,

$$\begin{aligned}\rho_1^{\star,n+1} &= \frac{1}{2}\rho_1^n + \frac{1}{2}\left[\rho_1^{\star,n+1} + \Delta t\,\boldsymbol{\nabla}\cdot\left(-\rho_1^{\star,n+1}\boldsymbol{v}^{\star,n+1} + \boldsymbol{F}^{\star,n+1}\right)\right]\\ \rho^{\star,n+1} &= \frac{1}{2}\rho^n + \frac{1}{2}\left[\rho^{\star,n+1} + \Delta t\,\boldsymbol{\nabla}\cdot\left(-\rho^{\star,n+1}\boldsymbol{v}^{\star,n+1}\right)\right].\end{aligned}$$

6. Calculate diffusive fluxes at the next time level (for lack of anything smarter, this seems most efficient),

$$\boldsymbol{F}^{n+1}=(\rho\chi\boldsymbol{\nabla}c)^{n+1}+\sqrt{\frac{2\left(\chi\rho\mu_c^{-1}\right)^{n+1}k_BT}{\Delta t\,\Delta V}}\,\widetilde{\boldsymbol{W}}^{n+1}.$$

In implementation, this may be postponed until the beginning of the next time step since it is the same as step 1 above.

7. Take a corrector step for velocity, using the same random fluxes as for the predictor stage (for lack of anything better),

$$\begin{aligned}
\frac{\rho^{n+1}\boldsymbol{v}^{n+1}-\rho^n\boldsymbol{v}^n}{\Delta t}+\boldsymbol{\nabla}\pi^{n+\frac{1}{2}} &= \frac{1}{2}\boldsymbol{\nabla}\cdot\left(-\rho^n\boldsymbol{v}^n\boldsymbol{v}^n-\rho^{\star,n+1}\boldsymbol{v}^{\star,n+1}\boldsymbol{v}^{\star,n+1}\right)+\frac{1}{2}\left(\rho^n+\rho^{n+1}\right)\boldsymbol{g}\\
&+ \frac{1}{2}\boldsymbol{\nabla}\cdot\left(\eta^n\bar{\boldsymbol{\nabla}}\boldsymbol{v}^n+\eta^{n+1}\bar{\boldsymbol{\nabla}}\boldsymbol{v}^{n+1}\right)+\boldsymbol{\nabla}\cdot\left[\sqrt{\frac{\eta^n k_BT}{\Delta t\,\Delta V}}\left(\boldsymbol{W}^n+(\boldsymbol{W}^n)^T\right)\right]\\
\boldsymbol{\nabla}\cdot\boldsymbol{v}^{n+1} &= S^{n+1}.
\end{aligned}$$

2 Overdamped Limit

The overdamped Eulerian dynamics can be efficiently simulated using the following Euler-Heun predictor-corrector temporal algorithm with time step size Δt, which updates the concentration from time step n to time step $n+1$ (denoted here by superscript):

1. Calculate predictor diffusive and stochastic fluxes,

$$\boldsymbol{F}^{n}=(\rho\chi\boldsymbol{\nabla}c)^{n}+\sqrt{\frac{2\left(\chi\rho\mu_c^{-1}\right)^{n}k_BT}{\Delta t\,\Delta V}}\,\widetilde{\boldsymbol{W}}^{n},$$

and then evaluate S^n from $\boldsymbol{F}^n$.

2. Generate a random advection velocity by solving the steady Stokes equation with random forcing,

$$\begin{aligned}
\boldsymbol{\nabla}\pi^{\star,n+1} &= \boldsymbol{\nabla}\cdot\left(\eta^n\bar{\boldsymbol{\nabla}}\boldsymbol{v}^{\star,n+1}\right)+\boldsymbol{\nabla}\cdot\left[\sqrt{\frac{\eta^n k_BT}{\Delta t\,\Delta V}}\left(\boldsymbol{W}^n+(\boldsymbol{W}^n)^T\right)\right]+\rho^n\boldsymbol{g}\\
\boldsymbol{\nabla}\cdot\boldsymbol{v}^{\star,n+1} &= S^n.
\end{aligned}$$

3. Take a predictor forward Euler step for ρ_1 and ρ,

$$\begin{aligned}
\rho_1^{\star,n+1} &= \rho_1^n+\Delta t\,\boldsymbol{\nabla}\cdot\left(-\rho_1^n\boldsymbol{v}^{\star,n+1}+\boldsymbol{F}^n\right)\\
\rho^{\star,n+1} &= \rho^n+\Delta t\,\boldsymbol{\nabla}\cdot\left(-\rho^n\boldsymbol{v}^{\star,n+1}\right).
\end{aligned}$$

4. Calculate corrector diffusive fluxes, and reuse the same random numbers,

$$\boldsymbol{F}^{\star,n+1}=(\rho\chi\boldsymbol{\nabla}c)^{\star,n+1}+\sqrt{\frac{2\left(\chi\rho\mu_c^{-1}\right)^{\star,n+1}k_BT}{\Delta t\,\Delta V}}\,\widetilde{\boldsymbol{W}}^{n}.$$

5. Solve the corrected steady Stokes equation

$$\begin{aligned}
\boldsymbol{\nabla}\pi^{n+\frac{1}{2}} &= \boldsymbol{\nabla}\cdot\left(\eta^{\star,n+1}\bar{\boldsymbol{\nabla}}\boldsymbol{v}^{n+1}\right)+\boldsymbol{\nabla}\cdot\left[\sqrt{\frac{\eta^n k_BT}{\Delta t\,\Delta V}}\left(\boldsymbol{W}^n+(\boldsymbol{W}^n)^T\right)\right]+\frac{1}{2}\left(\rho^n+\rho^{\star,n+1}\right)\boldsymbol{g}\\
\boldsymbol{\nabla}\cdot\boldsymbol{v}^{n+1} &= S^{\star,n+1}.
\end{aligned}$$

6. Update the densities and concentrations,

$$\begin{aligned}
\rho_1^{\star,n+1} &= \frac{1}{2}\rho_1^n+\frac{1}{2}\left[\rho_1^{\star,n+1}+\Delta t\,\boldsymbol{\nabla}\cdot\left(-\rho_1^{\star,n+1}\boldsymbol{v}^{n+1}+\boldsymbol{F}^{\star,n+1}\right)\right]\\
\rho^{\star,n+1} &= \frac{1}{2}\rho^n+\frac{1}{2}\left[\rho^{\star,n+1}+\Delta t\,\boldsymbol{\nabla}\cdot\left(-\rho^{\star,n+1}\boldsymbol{v}^{n+1}\right)\right].
\end{aligned}$$