Solving The Modified Diffusion Equation Using The Alternating Direction Implicit Method

In this note we will go over solving the modified diffusion equation, given in eq 0.1, using the Alternating Direction Implicit (ADI) method.

$$\frac{\partial q(\mathbf{r}, s)}{\partial s} = \frac{b^2}{6}\nabla^2 q(\mathbf{r}, s) - \omega(\mathbf{r})q(\mathbf{r}, s) \tag{0.1}$$

In the above equation, b is the Kuhn length of the polymers and $\omega(\mathbf{r})$ is the auxiliary field coupled to the polymer density. In eq 0.1, ∇^2 is the Laplacian operator, which could be written as

$$\begin{aligned}
&\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \quad \text{[Cartesian coordinates]},\\
&\nabla^2 \equiv \frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial}{\partial r}) + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2} + \frac{\partial^2}{\partial z^2} \quad \text{[Cylindrical coordinates]},\\
&\nabla^2 \equiv \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r}) + \frac{1}{r^2 sin^2\phi}\frac{\partial^2}{\partial \theta^2} + \frac{1}{r^2 sin\phi}\frac{\partial}{\partial \phi}(sin\phi\frac{\partial}{\partial \phi}) \quad \text{[Spherical coordinates]},
\end{aligned} \tag{0.2}$$

depending on the symmetry of the system. For sake of generality, we will write the Laplacian operator as $\nabla^2 \equiv \nabla_1 + \nabla_2 + \nabla_3$, where $(\nabla_1, \nabla_2, \nabla_3)$ can be defined depending on the dimensionality and symmetry of the system. In this note, we will be considering a two dimension system, with $\nabla^2 \equiv \nabla_1 + \nabla_2$. Using this notation, we can discretize the modified diffusion equation in two steps;

$$\frac{2}{\Delta s}[q_{ij}^{n+1/2} - q_{ij}^{n}] = \frac{b^2}{6}[\nabla_1 q_{ij}^{n+1/2} + \nabla_2 q_{ij}^{n}] - \frac{\omega_{ij}}{2}[q_{ij}^{n+1/2} + q_{ij}^{n}], \tag{0.3}$$

$$\frac{2}{\Delta s}[q_{ij}^{n+1} - q_{ij}^{n+1/2}] = \frac{b^2}{6}[\nabla_1 q_{ij}^{n+1/2} + \nabla_2 q_{ij}^{n+1}] - \frac{\omega_{ij}}{2}[q_{ij}^{n+1} + q_{ij}^{n+1/2}], \tag{0.4}$$

where i and j are indices running over the first and second dimension. For the purpose of this derivation, we will be considering the cylindrical coordinates, where

$$\begin{aligned}
\nabla_1 &\equiv \frac{1}{r}\frac{\partial}{\partial r} + \frac{\partial^2}{\partial r^2},\\
\nabla_2 &\equiv \frac{\partial^2}{\partial z^2}.
\end{aligned} \tag{0.5}$$

Applying the above operators to the modified diffusion equations 0.3 and 0.4 and solving for $q^{n+1/2}$

in terms of q^n and for q^{n+1} in terms of $q^{n+1/2}$, we get

$$q_{ij}^{n+1/2} - \frac{\Delta s b^2}{12}\Big[\frac{1}{i\Delta r + R}\frac{q_{i+1j}^{n+1/2} - q_{i-1j}^{n+1/2}}{2\Delta r} + \frac{q_{i+1j}^{n+1/2} - 2q_{ij}^{n+1/2} + q_{i-1j}^{n+1/2}}{\Delta r^2}\Big] + \frac{\Delta s \omega_{ij}}{4} q_{ij}^{n+1/2}$$
$$=$$
$$q_{ij}^{n} + \frac{\Delta s b^2}{12}\frac{q_{ij+1}^{n} - 2q_{ij}^{n} + q_{ij-1}^{n}}{\Delta z^2} - \frac{\Delta s \omega_{ij}}{4} q_{ij}^{n} \tag{0.6}$$

for the 1/2 step and

$$q_{ij}^{n+1} - \frac{\Delta s b^2}{12}\frac{q_{ij+1}^{n+1} - 2q_{ij}^{n+1} + q_{ij-1}^{n+1}}{\Delta z^2} - \frac{\Delta s \omega_{ij}}{4} q_{ij}^{n+1}$$
$$=$$
$$q_{ij}^{n+1/2} + \frac{\Delta s b^2}{12}\Big[\frac{1}{i\Delta r + R}\frac{q_{i+1j}^{n+1/2} - q_{i-1j}^{n+1/2}}{2\Delta r} + \frac{q_{i+1j}^{n+1/2} - 2q_{ij}^{n+1/2} + q_{i-1j}^{n+1/2}}{\Delta r^2}\Big] - \frac{\Delta s \omega_{ij}}{4} q_{ij}^{n+1/2} \tag{0.7}$$

In the above set of equations, R is the distance from the origin to the beginning of the calculation box. This is seen more clearly in figure 1. Further more, Δr and Δz are calculated by discretizing a box with dimensions of L_r and L_z in N_r and N_z points. For simplicity, we assume N_r=N_z=N.

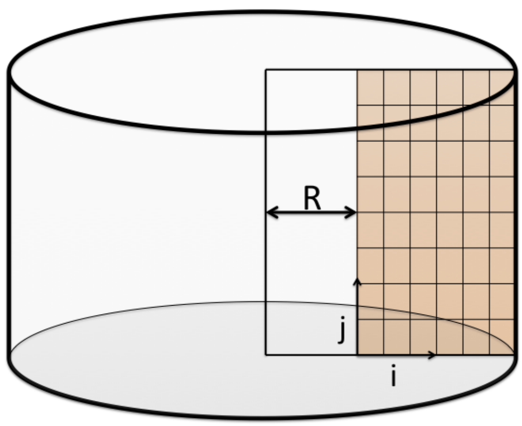

FIG. 1: A schematic diagram of the simulation box in the cylindrical geometry.

To simplify equations 0.6 and 0.7 we will introduce the following notation;

$$\alpha_i \equiv \frac{\Delta s b^2}{24\Delta r(i\Delta r + R)} - \frac{\Delta s b^2}{12\Delta r^2} \tag{0.8}$$

$$\beta_{ij} \equiv 1 + \frac{\Delta s \omega_{ij}}{4} + \frac{\Delta s b^2}{6\Delta r^2} \tag{0.9}$$

$$\gamma_i \equiv -\frac{\Delta s b^2}{24\Delta r(i\Delta r + R)} - \frac{\Delta s b^2}{12\Delta r^2} \tag{0.10}$$

$$\theta \equiv \frac{\Delta s b^2}{12\Delta z^2} \tag{0.11}$$

$$\sigma_{ij} \equiv 1 - \frac{\Delta s b^2}{6\Delta z^2} - \frac{\Delta s \omega_{ij}}{4} \tag{0.12}$$

$$\tag{0.13}$$

for the $n + 1/2$ step and

$$\hat{\theta} \equiv -\frac{\Delta s b^2}{12\Delta z^2} \tag{0.14}$$

$$\hat{\sigma}_{ij} \equiv 1 + \frac{\Delta s b^2}{6\Delta z^2} - \frac{\Delta s \omega_{ij}}{4} \tag{0.15}$$

$$\hat{\alpha}_i \equiv \frac{\Delta s b^2}{12\Delta r^2} - \frac{\Delta s b^2}{24\Delta r(i\Delta r + R)} \tag{0.16}$$

$$\hat{\beta}_{ij} \equiv 1 - \frac{\Delta s b^2}{6\Delta r^2} - \frac{\Delta s \omega_{ij}}{4} \tag{0.17}$$

$$\hat{\gamma}_i \equiv \frac{\Delta s b^2}{24\Delta r(i\Delta r + R)} + \frac{\Delta s b^2}{12\Delta r^2} \tag{0.18}$$

for the $n + 1$ step. Using the above notation, equations 0.6 and 0.7 can be written as

$$\alpha_i q_{i+1j}^{n+1/2} + \beta_{ij} q_{ij}^{n+1/2} + \gamma_i q_{i-1j}^{n+1/2} = \theta q_{ij-1}^{n} + \sigma_{ij} q_{ij}^{n} + \theta q_{ij+1}^{n} \tag{0.19}$$

$$\hat{\theta} q_{ij-1}^{n+1} + \hat{\sigma}_{ij} q_{ij}^{n+1} + \hat{\theta} q_{ij+1}^{n+1} = \hat{\alpha}_i q_{i-1j}^{n+1/2} + \hat{\beta}_{ij} q_{ij}^{n+1/2} + \hat{\gamma}_i q_{i+1j}^{n+1/2} \tag{0.20}$$

where we not yet consider the effect of boundary condition on the above set of equations. The choice of boundary condition depends on the specifics of the model examined. In our study, we apply the ADI method to bilayer forming block copolymers and thus we use the Neumann boundary condition, where ∇f=0.

In the matrix form, we can solve for $q^{n+1/2}$ for $0 < j < N-1$ using;

$$\begin{bmatrix} q_{0j}^{n+1/2} \\ q_{1j}^{n+1/2} \\ . \\ . \\ . \\ q_{N-1j}^{n+1/2} \end{bmatrix} = \begin{bmatrix} \beta_{0j} & (\gamma_0+\alpha_0) & 0 & . & . & 0 \\ \alpha_1 & \beta_{1j} & \gamma_1 & . & . & . \\ 0 & . & . & . & . & . \\ . & . & . & . & . & . \\ 0 & . & . & \alpha_{N-2} & \beta_{N-2j} & \gamma_{N-2} \\ 0 & . & . & . & (\gamma_{N-1}+\alpha_{N-1}) & \beta_{N-1j} \end{bmatrix}^{-1} \begin{bmatrix} \theta q_{0j-1}^n + \sigma_{0j} q_{0j}^n + \theta q_{0j+1}^n \\ \theta q_{1j-1}^n + \sigma_{1j} q_{1j}^n + \theta q_{1j+1}^n \\ . \\ . \\ . \\ \theta q_{N-1j-1}^n + \sigma_{N-1j} q_{N-1j}^n + \theta q_{N-1j+1}^n \end{bmatrix} \tag{0.21}$$

for j=0 using

$$\begin{bmatrix} q_{00}^{n+1/2} \\ q_{10}^{n+1/2} \\ . \\ . \\ . \\ q_{N-10}^{n+1/2} \end{bmatrix} = \begin{bmatrix} \beta_{00} & (\gamma_0+\alpha_0) & 0 & . & . & 0 \\ \alpha_1 & \beta_{10} & \gamma_1 & . & . & . \\ 0 & . & . & . & . & . \\ . & . & . & . & . & . \\ 0 & . & . & \alpha_{N-2} & \beta_{N-20} & \gamma_{N-2} \\ 0 & . & . & . & (\gamma_{N-1}+\alpha_{N-1}) & \beta_{N-10} \end{bmatrix}^{-1} \begin{bmatrix} \sigma_{00} q_{00}^n + 2\theta q_{01}^n \\ \sigma_{10} q_{10}^n + 2\theta q_{11}^n \\ . \\ . \\ . \\ \sigma_{N-10} q_{N-10}^n + 2\theta q_{N-11}^n \end{bmatrix} \tag{0.22}$$

and for j=N-1 using

$$\begin{bmatrix} q_{0N-1}^{n+1/2} \\ q_{1N-1}^{n+1/2} \\ . \\ . \\ . \\ q_{N-1N-1}^{n+1/2} \end{bmatrix} = \begin{bmatrix} \beta_{0N-1} & (\gamma_0+\alpha_0) & 0 & . & . & 0 \\ \alpha_1 & \beta_{1N-1} & \gamma_1 & . & . & . \\ 0 & . & . & . & . & . \\ . & . & . & . & . & . \\ 0 & . & . & \alpha_{N-2} & \beta_{N-2N-1} & \gamma_{N-2} \\ 0 & . & . & . & (\gamma_{N-1}+\alpha_{N-1}) & \beta_{N-1N-1} \end{bmatrix}^{-1} \begin{bmatrix} 2\theta q_{0N-2}^n + \sigma_{0N-1} q_{0N-1}^n \\ 2\theta q_{1N-2}^n + \sigma_{1N-1} q_{1N-1}^n \\ . \\ . \\ . \\ 2\theta q_{N-1N-2}^n + \sigma_{N-1N-1} q_{N-1N-1}^n \end{bmatrix} \tag{0.23}$$

where we have implemented the Neumann boundary condition in box i and j directions. Similarly, we can solve for q^{n+1} in the range $0 < i < N-1$ using,

$$\begin{bmatrix} q_{i0}^{n+1} \\ q_{i1}^{n+1} \\ . \\ . \\ . \\ q_{iN-1}^{n+1} \end{bmatrix} = \begin{bmatrix} \hat{\sigma}_{i0} & 2\hat{\theta} & 0 & . & . & 0 \\ \hat{\theta} & \hat{\sigma}_{i1} & \hat{\theta} & . & . & . \\ 0 & . & . & . & . & . \\ . & . & . & . & . & . \\ 0 & . & . & \hat{\theta} & \hat{\sigma}_{iN-2} & \hat{\theta} \\ 0 & . & . & . & 2\hat{\theta} & \hat{\sigma}_{iN-1} \end{bmatrix}^{-1} \begin{bmatrix} \hat{\alpha}_i q_{i-10}^{n+1/2} + \hat{\beta}_{i0} q_{i0}^{n+1/2} + \hat{\gamma}_i q_{i+10}^{n+1/2} \\ \hat{\alpha}_i q_{i-11}^{n+1/2} + \hat{\beta}_{i1} q_{i1}^{n+1/2} + \hat{\gamma}_i q_{i+11}^{n+1/2} \\ . \\ . \\ . \\ \hat{\alpha}_i q_{i-1N-1}^{n+1/2} + \hat{\beta}_{iN-1} q_{iN-1}^{n+1/2} + \hat{\gamma}_i q_{i+1N-1}^{n+1/2} \end{bmatrix} \tag{0.24}$$

and boundary point i=0 we write

$$\begin{bmatrix} q_{00}^{n+1} \\ q_{01}^{n+1} \\ . \\ . \\ . \\ q_{0N-1}^{n+1} \end{bmatrix} = \begin{bmatrix} \hat{\sigma}_{00} & 2\hat{\theta} & 0 & . & . & 0 \\ \hat{\theta} & \hat{\sigma}_{01} & \hat{\theta} & . & . & . \\ 0 & . & . & . & . & . \\ . & . & . & . & . & . \\ 0 & . & . & \hat{\theta} & \hat{\sigma}_{0N-2} & \hat{\theta} \\ 0 & . & . & . & 2\hat{\theta} & \hat{\sigma}_{0N-1} \end{bmatrix}^{-1} \begin{bmatrix} \hat{\beta}_{00} q_{00}^{n+1/2} + (\hat{\alpha}_0 + \hat{\gamma}_0) q_{10}^{n+1/2} \\ \hat{\beta}_{01} q_{01}^{n+1/2} + (\hat{\alpha}_0 + \hat{\gamma}_0) q_{11}^{n+1/2} \\ . \\ . \\ . \\ \hat{\beta}_{0N-1} q_{0N-1}^{n+1/2} + (\hat{\alpha}_0 + \hat{\gamma}_0) q_{1N-1}^{n+1/2} \end{bmatrix} \tag{0.25}$$

and for i=N-1 we can write

$$\begin{bmatrix} q_{N-10}^{n+1} \\ q_{N-11}^{n+1} \\ . \\ . \\ . \\ q_{N-1N-1}^{n+1} \end{bmatrix} = \begin{bmatrix} \hat{\sigma}_{N-10} & 2\hat{\theta} & 0 & . & . & 0 \\ \hat{\theta} & \hat{\sigma}_{N-11} & \hat{\theta} & . & . & . \\ 0 & . & . & . & . & . \\ . & . & . & . & . & . \\ 0 & . & . & \hat{\theta} & \hat{\sigma}_{N-1N-2} & \hat{\theta} \\ 0 & . & . & . & 2\hat{\theta} & \hat{\sigma}_{N-1N-1} \end{bmatrix}^{-1} \begin{bmatrix} \hat{\beta}_{N-10} q_{N-10}^{n+1/2} + (\hat{\alpha}_{N-1} + \hat{\gamma}_{N-1}) q_{N-20}^{n+1/2} \\ \hat{\beta}_{N-11} q_{N-11}^{n+1/2} + (\hat{\alpha}_{N-1} + \hat{\gamma}_{N-1}) q_{N-21}^{n+1/2} \\ . \\ . \\ . \\ \hat{\beta}_{N-1N-1} q_{N-1N-1}^{n+1/2} + (\hat{\alpha}_{N-1} + \hat{\gamma}_{N-1}) q_{N-2N-1}^{n+1/2} \end{bmatrix} \tag{0.26}$$

We solve the above set of equations $M-1$ times, where have assumed s can be discretized into $M-1$ steps of size Δs. For initial condition, we use $q_{ij}^{n=0}$=1.