The ADI method in 2-dimensional cylindrical coordinates (angular symmetry)

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The modified Diffusion Equation

We wish to solve a modified diffusion equation in a cylindrical coordinate system using the Alternating Direction Implicit (ADI) method. We assume angular symmetry, making our computational box two dimensional with indices in the radial (r) direction: $i = 0...N_r$, and the height (z) direction: $j = 0...N_z$. Instead of diffusion with respect to time, we are propagating along a continuous Gaussian chain representation of a polymer, where $q(\mathbf{r},\mathbf{z}, s)$ is an end integrated chain propagator and s is the index that runs along the length of the chain: $s = 0...N_s$. The modified diffusion equation has the form:

$$\frac{\partial q(\mathbf{r},\mathbf{z}; s)}{\partial s} = C\nabla^2 q(\mathbf{r},\mathbf{z}; s) - \omega(\mathbf{r},\mathbf{z})q(\mathbf{r},\mathbf{z}; s) \tag{1}$$

where C is the diffusion coefficient that represents R_g^2, the radius of gyration of the polymer squared, or $b^2/6$, where b is the persistence length of the polymer. The ω-field represents an auxiliary field coupled to polymer density. This calculation is performed in the cylindrical coordinate system, which means that the Laplacian has the form:

$$\nabla^2 = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial \Theta^2} + \frac{\partial^2}{\partial z^2} \tag{2}$$

Since we are assuming angular (Θ) symmetry, we remove the angular partial derivative from the Equation 2, and expand the radial component of the Laplacian:

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{\partial^2}{\partial z^2} \tag{3}$$

Inserting Equation 3 into the modified diffusion equation gives:

$$\frac{\partial q(\mathbf{r},\mathbf{z}; s)}{\partial s} = C\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{\partial^2}{\partial z^2}\right) q(\mathbf{r},\mathbf{z}; s) - \omega(\mathbf{r},\mathbf{z})q(\mathbf{r},\mathbf{z}; s) \tag{4}$$

Now that we have our modified diffusion equation in cylindrical coordinates with angular symmetry, we must define a computational grid of discrete points at which the continous function $q(\mathbf{r}, \mathbf{z}; s)$ can be sampled. Over the interval $\mathbf{r} \in [0, L_r]$, we use N_r equally spaced points:

$$r_i = i\Delta r, \quad i = 0...N_r - 1 \tag{5}$$

for $\Delta r = L_r/(N_r - 1)$, the chosen grid spacing in the r-direction. Over the interval $\mathbf{z} \in [0, L_z]$, we use N_z equally spaced points:

$$z_j = j\Delta z, \quad j = 0...N_z - 1 \tag{6}$$

for $\Delta z = L_z/(N_z - 1)$, the chosen grid spacing in the z-direction. We must also discretize the continous Gaussian chain over the interval $s \in [0, N]$ using N_s equally spaced points:

$$s_n = n\Delta s, \quad n = 0...N_s - 1 \tag{7}$$

for $\Delta s = N/(N_s - 1)$, the contour step along $q(r, z; s)$.

We now change our notation for the end-integrated chain propagator from it's continuous form, $q(r, z; s)$, to its discretized form, $q^n_{i,j}$ which we will use for the remainder of the derivation. As an initial condition, we set:

$$q^0_{i,j} = 1 \quad \text{for} \quad i \in [0, N_r - 1], \quad j \in [0, N_z - 1] \tag{8}$$

During the first step, we take a half step along s, and a step from i to $i + 1$ in the radial direction, while keeping the z-direction fixed.

$$q^n_{i,j} \to q^{n+1/2}_{i+1,j} \tag{9}$$

During the second step, we take the solution from the first step and solve the in z-direction while keeping the radial direction fixed.

$$q^{n+1/2}_{i+1,j} \to q^{n+1}_{i+1,j+1} \tag{10}$$

Step 1: Scan over r

The next step is to implement a finite differencing scheme to the modified diffusion equation. For the half s derivative, we use a forward Euler difference approximation:

$$\left.\frac{\partial q}{\partial s}\right|_{i,j;n} = \frac{q^{n+1/2}_{i,j} - q^n_{i,j}}{\Delta s/2} \tag{11}$$

For the first order r-derivative, we use a central difference approximation:

$$\left.\frac{\partial q}{\partial r}\right|_{i,j;n+1/2} = \frac{1}{2\Delta r}\left(q^{n+1/2}_{i+1,j} - q^{n+1/2}_{i-1,j}\right) \tag{12}$$

For the second order r-derivative and the second order z-derivative, we use another central difference approximation:

$$\left.\frac{\partial^2 q}{\partial r^2}\right|_{i,j;n+1/2} = \frac{1}{(\Delta r)^2}\left(q^{n+1/2}_{i+1,j} - 2q^{n+1/2}_{i,j} + q^{n+1/2}_{i-1,j}\right) \tag{13}$$

$$\left.\frac{\partial^2 q}{\partial z^2}\right|_{i,j;n} = \frac{1}{(\Delta z)^2}\left(q^n_{i,j+1} - 2q^n_{i,j} + q^n_{i,j-1}\right) \tag{14}$$

Aftern inserting the central difference approximations into the modified diffusion equation, the modified diffusion equation now has the form:

$$\frac{2}{\Delta s}(q^{n+1/2}_{i,j} - q^n_{i,j}) = \frac{C}{(\Delta r)^2}\left(q^{n+1/2}_{i+1,j} - 2q^{n+1/2}_{i,j} + q^{n+1/2}_{i-1,j}\right) + \frac{C}{2r\Delta r}\left(q^{n+1/2}_{i+1,j} - q^{n+1/2}_{i-1,j}\right) \tag{15}$$

$$+ \frac{C}{(\Delta z)^2}\left(q^n_{i,j+1} - 2q^n_{i,j} + q^n_{i,j-1}\right) - \omega_{i,j}\left(\frac{q^{n+1/2}_{i,j} + q^n_{i,j}}{2}\right) \tag{16}$$

The next step is to separate the n terms from the $n+1/2$ terms:

$$\frac{2}{\Delta s} q_{i,j}^{n+1/2} - \frac{C}{(\Delta r)^2}\left(q_{i+1,j}^{n+1/2} - 2q_{i,j}^{n+1/2} + q_{i-1,j}^{n+1/2}\right) - \frac{C}{2r\Delta r}\left(q_{i+1,j}^{n+1/2} - q_{i-1,j}^{n+1/2}\right) + \frac{1}{2}\omega_{i,j} q_{i,j}^{n+1/2} \tag{17}$$

$$= \frac{2}{\Delta s} q_{i,j}^{n} + \frac{C}{(\Delta z)^2}\left(q_{i,j+1}^{n} - 2q_{i,j}^{n} + q_{i,j-1}^{n}\right) - \frac{1}{2}\omega_{i,j} q_{i,j}^{n} \tag{18}$$

The next step is to group the coefficients by their coordinates (i,j). We multiply the entire expression by $\Delta s/2$ and use functions $\alpha_{1,0,-1}$ and $\beta_{1,0,-1}$ to simplify the expression:

$$\alpha_1 q_{i+1,j}^{n+1/2} + \alpha_0 q_{i,j}^{n+1/2} + \alpha_{-1} q_{i-1,j}^{n+1/2} = \beta_1 q_{i,j+1}^{n+1/2} + \beta_0 q_{i,j}^{n+1/2} + \beta_{-1} q_{i,j-1}^{n+1/2} \tag{19}$$

where:

$$\alpha_1 \equiv -\frac{C(\Delta s)}{2(\Delta r)^2} - \frac{C(\Delta s)}{4r(\Delta r)} \tag{20}$$

$$\alpha_0 \equiv 1 + \frac{C(\Delta s)}{(\Delta r)^2} + \frac{(\Delta s)}{4}\omega_{i,j} \tag{21}$$

$$\alpha_{-1} \equiv -\frac{C(\Delta s)}{2(\Delta r)^2} + \frac{C(\Delta s)}{4r(\Delta r)} \tag{22}$$

$$\beta_1 \equiv \frac{C(\Delta s)}{2(\Delta z)^2} \tag{23}$$

$$\beta_0 \equiv 1 - \frac{C(\Delta s)}{(\Delta z)^2} - \frac{(\Delta s)}{4}\omega_{i,j} \tag{24}$$

$$\beta_{-1} \equiv \frac{C(\Delta s)}{2(\Delta z)^2} \tag{25}$$

We implement a zero derivative boundary condition (Neumann boundary condition). The mathematical form of this boundary condition is the following:

$$\frac{\partial q_{0,j}}{\partial r} = \frac{\partial q_{N_r-1,j}}{\partial r} = \frac{\partial q_{i,0}}{\partial z} = \frac{\partial q_{i,N_z-1}}{\partial z} = 0 \tag{26}$$

Returning to the definition of the central difference approximation for the first partial derivative of r (or z), this requires that $q_{1,j} = q_{-1,j}$, $q_{N_r-2,j} = q_{N_r,j}$, $q_{i,1} = q_{i,-1}$, and $q_{i,N_z-2} = q_{i,N_z}$ for all s. We are now ready to write the first step of the ADI method in its matrix form. The idea behind this step is that we choose any $j \in [0, N_z-1]$, then solve in the r-direction. Typically we start with $j=0$, then increase j by one until we reach $j = N_z - 1$. There are three different j-cases that must be considered. The first case is$j=0$. In this case we are starting from the $(0,0)$ corner, and two boundary conditions apply. The matrix version of the modified diffusion equation is the following:

$$\begin{bmatrix} q_{0,0}^{n+1/2} \\ q_{1,0}^{n+1/2} \\ \vdots \\ q_{N_r-2,0}^{n+1/2} \\ q_{Nr-1,0}^{n+1/2} \end{bmatrix} = \begin{bmatrix} \alpha_0 & (\alpha_1+\alpha_{-1}) & 0 & \cdots & 0 \\ \alpha_{-1} & \alpha_0 & \alpha_{-1} & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & \alpha_{-1} & \alpha_0 & \alpha_1 \\ 0 & \cdots & 0 & (\alpha_1+\alpha_{-1}) & \alpha_0 \end{bmatrix}^{-1} \begin{bmatrix} 2\beta_1 q_{0,1}^n + \beta_0 q_{0,0}^n \\ 2\beta_1 q_{1,1}^n + \beta_0 q_{1,0}^n \\ \vdots \\ 2\beta_1 q_{N_r-2,1}^n + \beta_0 q_{N_r-2,0}^n \\ 2\beta_1 q_{N_r-1,1}^n + \beta_0 q_{N_r-1,0}^n \end{bmatrix}$$

The second case corresponds to $j \in 1...N_z - 2$, all the interior points. For this case, the matrix version of the modified diffusion equation is the following:

$$\begin{bmatrix} q_{0,0}^{n+1/2} \\ q_{1,0}^{n+1/2} \\ \vdots \\ q_{N_r-2,0}^{n+1/2} \\ q_{Nr-1,0}^{n+1/2} \end{bmatrix} = \begin{bmatrix} \alpha_0 & (\alpha_1+\alpha_{-1}) & 0 & \cdots & 0 \\ \alpha_{-1} & \alpha_0 & \alpha_{-1} & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & \alpha_{-1} & \alpha_0 & \alpha_1 \\ 0 & \cdots & 0 & (\alpha_1+\alpha_{-1}) & \alpha_0 \end{bmatrix}^{-1} \begin{bmatrix} \beta_1 q_{0,j+1}^n + \beta_0 q_{0,j}^n + \beta_{-1} q_{0,j-1}^n \\ \beta_1 q_{1,j+1}^n + \beta_0 q_{1,j}^n + \beta_{-1} q_{1,j-1}^n \\ \vdots \\ \beta_1 q_{N_r-2,j+1}^n + \beta_0 q_{N_r-2,j}^n + \beta_{-1} q_{N_r-2,j-1}^n \\ \beta_1 q_{N_r-1,j+1}^n + \beta_0 q_{N_r-1,j}^n + \beta_{-1} q_{N_r-1,j-1}^n \end{bmatrix}$$

The third case is if $j = N_z - 1$. Similarly to the first case, we are in a corner and two boundary conditions apply. In this case, the matrix version of the modified diffusion equation is:

$$\begin{bmatrix} q_{0,0}^{n+1/2} \\ q_{1,0}^{n+1/2} \\ \vdots \\ q_{N_r-2,0}^{n+1/2} \\ q_{Nr-1,0}^{n+1/2} \end{bmatrix} = \begin{bmatrix} \alpha_0 & (\alpha_1+\alpha_{-1}) & 0 & \cdots & 0 \\ \alpha_{-1} & \alpha_0 & \alpha_{-1} & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & \alpha_{-1} & \alpha_0 & \alpha_1 \\ 0 & \cdots & 0 & (\alpha_1+\alpha_{-1}) & \alpha_0 \end{bmatrix}^{-1} \begin{bmatrix} 2\beta_{-1} q_{0,N_z-2}^n + \beta_0 q_{0,N_z-1}^n \\ 2\beta_{-1} q_{1,N_z-2}^n + \beta_0 q_{1,N_z-1}^n \\ \vdots \\ 2\beta_{-1} q_{N_r-2,N_z-2}^n + \beta_0 q_{N_r-2,N_z-1}^n \\ 2\beta_{-1} q_{N_r-1,N_z-2}^n + \beta_0 q_{N_r-1,N_z-1}^n \end{bmatrix}$$

In all three cases, this matrix algebra problem can be solved efficiently using a tridiagonal matrix algorithm (TDMA) in $O(N_r)$ steps. After scanning over the r-direction for all j, we now move to step 2, from $n+1/2$ to $n+1$.

Step 2: Scan over z

Much of this section is similar to Step 1. However, there are a few small differences resulting from the use of the Laplacian operator in 2 dimensional cylindrical coordinates. Similarly to Step 1, we use a forward Euler difference approximation for the second half s derivative:

$$\left.\frac{\partial q}{\partial s}\right|_{i,j;n} = \frac{q_{i,j}^{n+1} - q_{i,j}^{n+1/2}}{\Delta s/2} \tag{27}$$

We keep the radial direction stationary, so the r-derivatives are the same. See Equations 11 and 12. The second order z derivative changes to:

$$\left.\frac{\partial^2 q}{\partial z^2}\right|_{i,j;n} = \frac{1}{(\Delta z)^2}\left(q_{i,j+1}^{n+1} - 2q_{i,j}^{n+1} + q_{i,j-1}^{n+1}\right) \tag{28}$$

The modified diffusion equation now has the form:

$$\frac{2}{\Delta s}(q_{i,j}^{n+1} - q_{i,j}^{n+1/2}) = \frac{C}{(\Delta r)^2}\left(q_{i+1,j}^{n+1/2} - 2q_{i,j}^{n+1/2} + q_{i-1,j}^{n+1/2}\right) + \frac{C}{2r\Delta r}\left(q_{i+1,j}^{n+1/2} - q_{i-1,j}^{n+1/2}\right) \tag{29}$$

$$= + \frac{C}{(\Delta z)^2}\left(q_{i,j+1}^{n+1} - 2q_{i,j}^{n+1} + q_{i,j-1}^{n+1}\right) - \omega_{i,j}\left(\frac{q_{i,j}^{n+1} + q_{i,j}^{n+1/2}}{2}\right) \tag{30}$$

The next step is to separate the $n+1$ terms from the $n+1/2$ terms:

$$\frac{2}{\Delta s}q_{i,j}^{n+1} - \frac{C}{(\Delta z)^2}\left(q_{i,j+1}^{n+1} - 2q_{i,j}^{n+1} + q_{i,j-1}^{n+1}\right) + \frac{\omega_{i,j}}{2}q_{i,j}^{n+1} \tag{31}$$

$$= \frac{2}{\Delta s}q_{i,j}^{n+1/2} + \frac{C}{(\Delta r)^2}\left(q_{i+1,j}^{n+1/2} - 2q_{i,j}^{n+1/2} + q_{i-1,j}^{n+1/2}\right) + \frac{C}{2r\Delta r}\left(q_{i+1,j}^{n+1/2} - q_{i-1,j}^{n+1/2}\right) - \frac{\omega_{i,j}}{2}q_{i,j}^{n+1/2} \tag{32}$$

The next step is to group the coefficients by their coordinates (i,j). We multiply the entire expression by $\Delta s/2$ and use functions $\gamma_{1,0,-1}$ and $\sigma_{1,0,-1}$ to simplify the expression:

$$\gamma_1 q_{i,j+1}^{s+1} + \gamma_0 q_{i,j}^{s+1} + \gamma_{-1} q_{i,j-1}^{s+1} = \sigma_1 q_{i+1,j}^{s+1/2} + \sigma_0 q_{i,j}^{s+1/2} + \sigma_{-1} q_{i-1,j}^{s+1/2} \tag{33}$$

where the γ and σ functions are:

$$\gamma_1 \equiv -\frac{C(\Delta s)}{2(\Delta z)^2} \tag{34}$$

$$\gamma_0 \equiv 1 + \frac{C(\Delta s)}{(\Delta z)^2} + \frac{(\Delta s)}{4}\omega_{i,j} \tag{35}$$

$$\gamma_{-1} \equiv -\frac{C(\Delta s)}{2(\Delta z)^2} \tag{36}$$

$$\sigma_1 \equiv \frac{C(\Delta s)}{2(\Delta r)^2} + \frac{C(\Delta s)}{4r(\Delta r)} \tag{37}$$

$$\sigma_0 \equiv 1 - \frac{C(\Delta s)}{(\Delta r)^2} - \frac{(\Delta s)}{4}\omega_{i,j} \tag{38}$$

$$\sigma_{-1} \equiv \frac{C(\Delta s)}{2(\Delta r)^2} - \frac{C(\Delta s)}{4r(\Delta r)} \tag{39}$$

We are implementing a zero-derivative boundary condition in our computational box. During this step, we choose any i, and solve in the j direction. Identically to step 1, there are three cases. In the first case, $i=0$. The matrix formulation for the modified diffusion equation has the following form:

$$\begin{bmatrix} q_{0,0}^{n+1} \\ q_{0,1}^{n+1} \\ \vdots \\ q_{0,N_z-2}^{n+1} \\ q_{0,N_z-1}^{n+1} \end{bmatrix} = \begin{bmatrix} \gamma_0 & 2\gamma_1 & 0 & \cdots & 0 \\ \gamma_{-1} & \gamma_0 & \gamma_{-1} & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & \gamma_{-1} & \gamma_0 & \gamma_1 \\ 0 & \cdots & 0 & 2\gamma_1 & \gamma_0 \end{bmatrix}^{-1} \begin{bmatrix} (\sigma_1+\sigma_{-1})q_{1,0}^{n+1/2} + \sigma_0 q_{0,0}^{n+1/2} \\ (\sigma_1+\sigma_{-1})q_{1,1}^{n+1/2} + \sigma_0 q_{0,1}^{n+1/2} \\ \vdots \\ (\sigma_1+\sigma_{-1})q_{1,N_z-2}^{n+1/2} + \sigma_0 q_{0,N_z-2}^{n+1/2} \\ (\sigma_1+\sigma_{-1})q_{1,N_z-1}^{n+1/2} + \sigma_0 q_{0,N_z-1}^{n+1/2} \end{bmatrix}$$

The second case is if we choose $i \in 1 \cdots N_z - 2$. This corresponds to all the interior points. For this case, the matrix version of the modified diffusion equation is the following:

$$\begin{bmatrix} q_{i,0}^{n+1} \\ q_{i,1}^{n+1} \\ \vdots \\ q_{i,N_z-2}^{n+1} \\ q_{i,N_z-1}^{n+1} \end{bmatrix} = \begin{bmatrix} \gamma_0 & 2\gamma_1 & 0 & \cdots & 0 \\ \gamma_{-1} & \gamma_0 & \gamma_{-1} & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & \gamma_{-1} & \gamma_0 & \gamma_1 \\ 0 & \cdots & 0 & 2\gamma_1 & \gamma_0 \end{bmatrix}^{-1} \begin{bmatrix} \sigma_1 q_{i+1,0}^{n+1/2} + \sigma_0 q_{i,0}^{n+1/2} + \sigma_{-1} q_{i-1,0}^{n+1/2} \\ \sigma_1 q_{i+1,1}^{n+1/2} + \sigma_0 q_{i,1}^{n+1/2} + \sigma_{-1} q_{i-1,1}^{n+1/2} \\ \vdots \\ \sigma_1 q_{i+1,N_z-2}^{n+1/2} + \sigma_0 q_{i,N_z-2}^{n+1/2} + \sigma_{-1} q_{i-1,N_z-2}^{n+1/2} \\ \sigma_1 q_{i+1,N_z-1}^{n+1/2} + \sigma_0 q_{i,N_z-1}^{n+1/2} + \sigma_{-1} q_{i-1,N_z-1}^{n+1/2} \end{bmatrix}$$

The third case is if we choose j = $N_z - 1$. Similarly to the first case, we start in a corner where two boundary conditions apply. In this case, the matrix version of the modified diffusion equation is:

$$\begin{bmatrix} q_{0,0}^{n+1} \\ q_{0,1}^{n+1} \\ \vdots \\ q_{0,N_z-2}^{n+1} \\ q_{0,N_z-1}^{n+1} \end{bmatrix} = \begin{bmatrix} \gamma_0 & 2\gamma_1 & 0 & \cdots & 0 \\ \gamma_{-1} & \gamma_0 & \gamma_{-1} & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & \gamma_{-1} & \gamma_0 & \gamma_1 \\ 0 & \cdots & 0 & 2\gamma_1 & \gamma_0 \end{bmatrix}^{-1} \begin{bmatrix} (\sigma_1+\sigma_{-1})q_{N_r-2,0}^{n+1/2} + \sigma_0 q_{N_r-1,0}^{n+1/2} \\ (\sigma_1+\sigma_{-1})q_{N_r-2,1}^{n+1/2} + \sigma_0 q_{N_r-1,1}^{n+1/2} \\ \vdots \\ (\sigma_1+\sigma_{-1})q_{N_r-2,N_z-2}^{n+1/2} + \sigma_0 q_{N_r-1,N_z-2}^{n+1/2} \\ (\sigma_1+\sigma_{-1})q_{N_r-2,N_z-1}^{n+1/2} + \sigma_0 q_{N_r-1,N_z-1}^{n+1/2} \end{bmatrix}$$

We solve these matrix algebra problems with the TDMA algorithm. After scanning over the z-direction for all i, we are at the end of the two step ADI process and have moved along the chain from n to $n+1$. The next step is to repeat steps 1 and 2 along the length of the Gaussian chain until we reach $n = N_s - 1$.