Efficient computation of the order parameter and director field

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Suppose we know the Q tensor components at every point in space. The order parameter is defined as the largest eigenvalue of Q, and the director field the corresponding eigenvector.

The Q tensor is both traceless and symmetric, and so we can write it as

$$Q = \begin{pmatrix} Q_{xx} & Q_{xy} & Q_{xz} \\ Q_{xy} & Q_{yy} & Q_{yz} \\ Q_{xz} & Q_{yz} & -Q_{xx} - Q_{yy} \end{pmatrix}.$$

The most intuitive approach is to check every point in space and diagonalize Q, at which point we obtain both the eigenvalues and eigenvectors and can uniquely identify the order parameter and director field. However, this approach is slow, since we cannot necessarily diagonalize Q at every point in space simultaneously. We instead seek a solution that can be readily parallelized.

We know that the eigenvalues are the roots of the characteristic polynomial

$$P(\lambda) = \det(\lambda I - Q).$$

Since Q is traceless and symmetric, this equation takes the relatively simple form

$$P(\lambda) = \lambda^3 - \frac{1}{2}\operatorname{tr}\left(Q^2\right)\lambda - \frac{1}{3}\operatorname{tr}\left(Q^3\right) = \lambda^3 - p\lambda - q$$

where we have defined

$$p = \frac{1}{2}\operatorname{tr}\left(Q^2\right) \quad \text{and} \quad q = \frac{1}{3}\operatorname{tr}\left(Q^3\right) = \det(Q).$$

Note that $p \geq 0$ since it is the sum of squares of real eigenvalues (the fact that the eigenvalues are real is guaranteed since Q is Hermitian). However, we don't necessarily know the sign of q.

Let $\lambda = r\cos\theta$. Then we have that

$$\lambda^3 = r^3\cos^3\theta = \frac{1}{4}r^3[3\cos\theta + \cos 3\theta] = \frac{3r^3}{4}\lambda + \frac{r^3}{4}\cos 3\theta.$$

The cubic can therefore be written as

$$\frac{r^3}{4}\cos(3\theta) + \left(\frac{3r^3}{4} - pr\right)\cos\theta = q.$$

Now, choose $r = 2\sqrt{p/3}$. Then this reduces to

$$\cos(3\theta) = 4q/r^3.$$

from which we find

$$\lambda_k = r\cos\left(\frac{1}{3}\arccos\Big(4q/r^3\Big) + 2\pi k/3\right).$$

Note that arccos(x) function only returns real numbers if $|x| \leq 1$, and therefore there is the condition

$$27q^2 \leq 4p^3.$$

If this condition holds, then we can guarantee that $\lambda_0 \geq \lambda_1 \geq \lambda_2$. Since we know the eigenvalues of Q must be real, this condition is already guaranteed; however, we'll look at this explicitly for completeness. For the Q tensor, this condition is

$$54\det(Q)^2 = 54\lambda_0^2\lambda_1^2\lambda_2^2 \leq \operatorname{tr}\Big(Q^2\Big)^3 = (\lambda_0^2 + \lambda_1^2 + \lambda_2^2)^3.$$

Using the fact that $\operatorname{tr}(Q) = \lambda_0 + \lambda_1 + \lambda_2 = 0$, this can be reduced to find

$$(\lambda_0 - \lambda_1)^2(2\lambda_0 + \lambda_1)^2(\lambda_0 + 2\lambda_1)^2 \geq 0.$$

This clearly holds for any real eigenvalues.

We now seek to find the director field. We know that $\boldsymbol{n}$ satisfies the equation

$$Q \cdot \boldsymbol{n} = \lambda_0 \boldsymbol{n}.$$

In full, this is

$$\begin{pmatrix} (Q_{xx} - \lambda_0)n_x + Q_{xy}n_y + Q_{xz}n_z \\ Q_{xy}n_x + (Q_{yy} - \lambda_0)n_y + Q_{yz}n_z \\ Q_{xz}n_x + Q_{yz}n_y - (Q_{xx} + Q_{yy} + \lambda_0)n_z \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}.$$

We can solve this to find that

$$n \propto \begin{pmatrix} Q_{xz}(Q_{yy} - \lambda_0) - Q_{xy}Q_{yz} \\ Q_{yz}(Q_{xx} - \lambda_0) - Q_{xy}Q_{xz} \\ Q_{xy}^2 - (Q_{xx} - \lambda_0)(Q_{yy} - \lambda_0) \end{pmatrix}.$$

After normalization, we will have the director field everywhere.

To summarize, we can easily find the largest eigenvalue of Q to be

$$\lambda_0 = r\cos\left(\frac{1}{3}\arccos\Big(4q/r^3\Big)\right)$$

where $r = 2\sqrt{p/3}$ and

$$p = \frac{1}{2}\operatorname{tr}\Big(Q^2\Big) \quad \text{and} \quad q = \det(Q).$$

Since these coefficients can be determined at every point in space simultaneously, the largest eigenvalue S can also be determined at every point in space very efficiently. Once S is known, the computation of the director field can be performed easily, giving us n and S without needing to diagonalize Q.

Note that if Q is defined as

$$Q = \alpha S(3\boldsymbol{nn} - I),$$

then $\lambda_0 = 2\alpha S$, and so $\lambda_1 + \lambda_2 = -2\alpha S$. Common choices for α are $1/2$ or $1/3$. The biaxial order parameter b is found via

$$b = |\lambda_1 - \lambda_2|/2\alpha.$$

That is, we often take $\lambda_1 = -\alpha(S - b)$ and $\lambda_2 = -\alpha(S + b)$, where $b \geq 0$.