3.21 Problem Set 1

Homework Group:  

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Problem G 1.1

We are given a function $c = A(xy + yz + zx)$, with $A =$ constant.

(a) We want to find cosines of the direction in which $c$ changes most rapidly with distance from point $P = (1,1,1)$. The direction of most rapid change is the gradient of $c$:

$$\nabla c = A[(y + z)i + (x + z)j + (x + y)k].$$

At point $P$, the gradient is

$$\nabla c = A[2i + 2j + 2k].$$

For a vector $\vec{B}$, the directional cosine to a unit vector $\hat{i}$ is given by

$$\cos \theta = \frac{\vec{B} \cdot \hat{i}}{|\vec{B}|}.$$  

We know that the magnitude of our vector is

$$|\nabla c| = 2A\sqrt{3}.$$
Thus, for all three directions in the Cartesian plane $(\hat{i}, \hat{j}, \hat{k})$, the directional cosine is

$$\cos \theta = \frac{2A}{2A\sqrt{3}} = \frac{1}{\sqrt{3}} = \frac{\sqrt{3}}{3},$$

because $|\hat{i}| = |\hat{j}| = |\hat{k}| = 1$.

(b) We want the maximum rate of change of $c$ at $P$. This is simply equal to the magnitude of $c$ in the direction of the maximum rate of change; in other words, the magnitude of the gradient.

$$|\nabla c| = 2A\sqrt{3}$$

![Gradient Field Diagram](image)

Figure 1: A plot of the gradient field: the lower front corner is the origin, and the vector magnitude increases in the $1, 1, 1$ direction.

**Problem G 1.2**

Given a field $\vec{J} = A(x\hat{i} + y\hat{j})$, with $A = \text{constant}$, and using the Divergence Theorem we
find the flow rate to be

$$\hat{M}_i = \int_{\Delta V} \nabla \cdot \vec{J}_i \, dV.$$ 

where

$$\nabla \cdot \vec{J} = \frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} + \frac{\partial J_z}{\partial z} = \Lambda(1 + 1 + 0) = 2A.$$ 

Since $\nabla \cdot \vec{J}$ is a constant, we can evaluate the volume integral as follows:

$$\hat{M}_i = \int_{\Delta V} 2AdV = 2A \int_{\Delta V} dV,$$

and because the volume of half a unit sphere is $\frac{4}{3}\pi$,

$$\hat{M}_i = \frac{2A4\pi}{6} = \frac{4}{3}A\pi.$$ 

**Problem G 1.3**

See attached output from Mathematica.

**Problem G 1.4**

(a) *Indicate the relationship between Onsager coefficients and features on the graph.*

Allowing coupling between the temperature and charge fields, the heat and charge flux are given by:

$$J_Q = \frac{-L_{QQ}}{T} \nabla T - L_{Q\phi} \nabla \phi,$$

$$J_q = -L_{q\phi} \nabla \phi - \frac{L_{qQ}}{T} \nabla T,$$

respectively. The charge potential may be related to the imposed electric field, $E$, by

$$E = -\nabla \phi.$$ 

Substituting this expression as the driving force for charge flux gives:

$$J_Q = \frac{-L_{QQ}}{T} \nabla T + L_{Q\phi} E \tag{1}$$
Question G1–3

dNa = -(kac + kab) Na + kba Nb + kca Nc
dNb = kab Na - (kbc + kba) Nb + kcb Nc
dNc = kac Na + kbc Nb - (kca + kcb) Nc

(-kab - kac) Na + kba Nb + kca Nc
kab Na - (kbc + kba) Nb + kcb Nc
kac Na + kbc Nb - (kca + kcb) Nc

\[ x = \text{Solve} \{ \begin{align*}
& \{ (\text{dNa} = 0, \text{dNb} = 0, \text{dNc} = 0, \text{Na} + \text{Nb} + \text{Nc} = \text{Nt}) \}, \{ \text{Na}, \text{Nb}, \text{Nc} \} \} \\
& \{ (\text{Na} \rightarrow -(\text{kac kca Nt} - \text{kbc kca Nt} - \text{kba kcb Nt}) / \\
& \quad (\text{kac kba + kab kbc + kac kbc + kac kca + kba kca + kbc kca + kab kcb + kac kcb + kba kcb}), \\
& \text{Nb} \rightarrow -(\text{kac kca Nt} - \text{kab kbc Nt} - \text{kac kcb Nt}) / \\
& \quad (\text{kac kba + kab kbc + kac kbc + kac kca + kba kca + kbc kca + kab kcb + kac kcb + kba kcb}), \\
& \text{Nc} \rightarrow -(\text{kac kba Nt} - \text{kab kbc Nt} - \text{kac kcb Nt}) / \\
& \quad (\text{kac kba + kab kbc + kac kbc + kac kca + kba kca + kbc kca + kab kcb + kac kcb + kba kcb}) \} \} \\
\]

Na = -(\text{kac kca Nt} - \text{kbc kca Nt} - \text{kba kcb Nt}) / \\
(\text{kac kba + kab kbc + kac kbc + kac kca + kba kca + kbc kca + kab kcb + kac kcb + kba kcb});

\text{Nb} = -(\text{kac kca Nt} - \text{kab kbc Nt} - \text{kac kcb Nt}) / \\
(\text{kac kba + kab kbc + kac kbc + kac kca + kba kca + kbc kca + kab kcb + kac kcb + kba kcb});

\text{Nc} = -(\text{kac kba Nt} - \text{kab kbc Nt} - \text{kac kcb Nt}) / \\
(\text{kac kba + kab kbc + kac kbc + kac kca + kba kca + kbc kca + kab kcb + kac kcb + kba kcb});

\text{Na} / \text{Nb} // \text{Simplify}

\begin{align*}
\text{kbc kca + kba (kca + kcb)} \\
\text{kac kcb + kab (kca + kcb)}
\end{align*}

\text{Nb} / \text{Nc} // \text{Simplify}

\begin{align*}
\text{kac kcb + kab (kca + kcb)} \\
\text{kab kbc + kac (kba + kbc)}
\end{align*}

\text{Nc} / \text{Na} // \text{Simplify}

\begin{align*}
\text{kab kbc + kac (kba + kbc)} \\
\text{kbc kca + kba (kca + kcb)}
\end{align*}

The right half of Equation 2.51 is verified! However the left half contains an error.

For example, at equilibrium the rate from A to B must equal the rate from B to A. Assuming a simple first order kinetic relationship Na[kab]=Nb[kba]; thus

\[ \frac{\text{Na}}{\text{Nb}} = \frac{\text{kkb}}{\text{kacb}} \]

which is the inverse of what is written in the book.