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MATEMATIKA KIMIA
Lampiran
Transformasi operator del menjadi koordinat sferis terkutub

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TRANSFORMATION OF ∇^2 TO SPHERICAL POLAR COORDINATES

The Laplacian operator has its simplest form in Cartesian coordinates

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

The transformation and reverse transformation equations from Cartesian to spherical polar coordinates are

$$x = r\sin\theta\cos\phi \qquad r = (x^2+y^2+z^2)^{1/2}$$

$$y = r\sin\theta\sin\phi \qquad \cos\theta = \frac{z}{(x^2+y^2+z^2)^{1/2}}$$

$$z = r\cos\theta \qquad \tan\phi = \frac{y}{x}$$

We now must determine the transformation derivatives:

$$\frac{\partial r}{\partial x} = \frac{1}{2}(x^2+y^2+z^2)^{-1/2}2x = \frac{x}{r} = \sin\theta\cos\phi$$

Likewise,

$$\frac{\partial r}{\partial y} = \sin\theta\sin\phi; \quad \frac{\partial r}{\partial z} = \cos\theta$$

A simple way to find $\partial\theta/\partial x$ without having to differentiate the inverse cosine is to differentiate $\cos\theta$ directly.

$$-\sin\theta\, d\theta = -z\left(\frac{1}{2}\right)(x^2+y^2+z^2)^{-3/2}(2x)\,dx = -\frac{zx}{r^3}\,dx$$

$$-d\theta = -\frac{\cos\phi\cos\theta}{r}\,dx$$

$$\frac{\partial\theta}{\partial x} = \frac{\cos\phi\cos\theta}{r}$$

By the same method, we have

$$\frac{\partial\theta}{\partial y} = \frac{\sin\phi\cos\theta}{r} \quad \text{and} \quad \frac{\partial\theta}{\partial z} = \frac{-\sin\theta}{r}$$

To find $\partial\phi/\partial x$ we differentiate the tangent ϕ directly.

$$\sec^2\phi\, d\phi = -\frac{y}{x^2}\,dx$$

$$\frac{d\phi}{\cos^2\phi} = -\frac{r\sin\theta\sin\phi\,dx}{r^2\sin^2\theta\cos^2\phi}$$

$$\frac{\partial\phi}{\partial x} = -\frac{\sin\phi}{r\sin\theta}$$

Likewise,

$$\frac{\partial\phi}{\partial y} = \frac{\cos\phi}{r\sin\theta} \quad \text{and} \quad \frac{\partial\phi}{\partial z} = 0$$

The transformation equations for the first derivatives are found using the chain rule.

$$\frac{\partial}{\partial x} = \frac{\partial r}{\partial x}\frac{\partial}{\partial r} + \frac{\partial\theta}{\partial x}\frac{\partial}{\partial\theta} + \frac{\partial\phi}{\partial x}\frac{\partial}{\partial\phi}$$

$$\frac{\partial}{\partial x} = \sin\theta\cos\phi\frac{\partial}{\partial r} + \frac{\cos\phi\cos\theta}{r}\frac{\partial}{\partial\theta} - \frac{\sin\phi}{r\sin\theta}\frac{\partial}{\partial\phi}$$

$$\frac{\partial}{\partial y} = \frac{\partial r}{\partial y}\frac{\partial}{\partial r} + \frac{\partial\theta}{\partial y}\frac{\partial}{\partial\theta} + \frac{\partial\phi}{\partial y}\frac{\partial}{\partial\phi}$$

$$\frac{\partial}{\partial y} = \sin\theta\sin\phi\frac{\partial}{\partial r} + \frac{\sin\phi\cos\theta}{r}\frac{\partial}{\partial\theta} + \frac{\cos\phi}{r\sin\theta}\frac{\partial}{\partial\phi}$$

$$\frac{\partial}{\partial z} = \frac{\partial r}{\partial z}\frac{\partial}{\partial r} + \frac{\partial\theta}{\partial z}\frac{\partial}{\partial\theta} + \frac{\partial\phi}{\partial z}\frac{\partial}{\partial\phi}$$

$$\frac{\partial}{\partial z} = \cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial\theta}$$

To find the second derivatives of these operators, we now must operate each operator on itself. Remember that when $\sin\theta\cos\phi\,\partial/\partial r$ operates on $(\cos\phi\cos\theta/r)\,\partial/\partial\theta$, only the $\cos\phi\cos\theta$ passes through the $\partial/\partial r$ operator. The term $(1/r)(\partial/\partial\theta)$ must be differentiated as a product.

$$\begin{aligned}
\frac{\partial}{\partial x}\frac{\partial}{\partial x} = {} & \sin^2\theta\cos^2\phi\frac{\partial^2}{\partial r^2} + \frac{\sin\theta\cos\theta\cos^2\phi}{r}\frac{\partial^2}{\partial r\,\partial\theta} - \frac{\sin\theta\cos\theta\cos^2\phi}{r^2}\frac{\partial}{\partial\theta} \\
& - \frac{\sin\phi\cos\phi}{r}\frac{\partial^2}{\partial r\,\partial\phi} + \frac{\sin\phi\cos\phi}{r^2}\frac{\partial}{\partial\phi} + \frac{\cos\theta\cos^2\phi\sin\theta}{r}\frac{\partial^2}{\partial\theta\,\partial r} \\
& + \frac{\cos^2\phi\cos^2\theta}{r}\frac{\partial}{\partial r} + \frac{\cos^2\phi\cos^2\theta}{r^2}\frac{\partial^2}{\partial\theta^2} - \frac{\sin\theta\cos\theta\cos^2\phi}{r^2}\frac{\partial}{\partial\theta} \\
& - \frac{\sin\phi\cos\phi\cos\theta}{r^2\sin\theta}\frac{\partial^2}{\partial\theta\,\partial\phi} + \frac{\sin\phi\cos\phi\cos^2\theta}{r^2\sin^2\theta}\frac{\partial}{\partial\phi} - \frac{\sin\phi\cos\phi}{r}\frac{\partial^2}{\partial\phi\,\partial r} \\
& + \frac{\sin^2\phi}{r}\frac{\partial}{\partial r} - \frac{\sin\phi\cos\phi\cos\theta}{r^2\sin\theta}\frac{\partial^2}{\partial\phi\,\partial r} + \frac{\sin^2\phi\cos\theta}{r^2\sin\theta}\frac{\partial}{\partial\theta} \\
& + \frac{\sin^2\phi}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{\sin\phi\cos\phi}{r^2\sin^2\theta}\frac{\partial}{\partial\phi}
\end{aligned}$$

$$\frac{\partial}{\partial y}\frac{\partial}{\partial y} = \sin^2\theta\sin^2\phi\frac{\partial^2}{\partial r^2} + \frac{\sin\theta\cos\theta\sin^2\phi}{r}\frac{\partial^2}{\partial r\,\partial\theta} - \frac{\sin\theta\cos\theta\sin^2\phi}{r^2}\frac{\partial}{\partial\theta}$$
$$+ \frac{\sin\phi\cos\phi}{r}\frac{\partial^2}{\partial r\,\partial\phi} - \frac{\sin\phi\cos\phi}{r^2}\frac{\partial}{\partial\phi} + \frac{\cos\theta\sin^2\phi\sin\theta}{r}\frac{\partial^2}{\partial\theta\,\partial r}$$
$$+ \frac{\sin^2\phi\cos^2\theta}{r}\frac{\partial}{\partial r} + \frac{\sin^2\phi\cos^2\theta}{r^2}\frac{\partial^2}{\partial\theta^2} - \frac{\sin\theta\cos\theta\sin^2\phi}{r^2}\frac{\partial}{\partial\theta}$$
$$+ \frac{\sin\phi\cos\phi\cos\theta}{r^2\sin\theta}\frac{\partial^2}{\partial\theta\,\partial\phi} - \frac{\sin\phi\cos\phi\cos^2\theta}{r^2\sin^2\theta}\frac{\partial}{\partial\phi} + \frac{\sin\phi\cos\phi}{r}\frac{\partial^2}{\partial\phi\,\partial r}$$
$$+ \frac{\cos^2\phi}{r}\frac{\partial}{\partial r} + \frac{\sin\phi\cos\phi\cos\theta}{r^2\sin\theta}\frac{\partial^2}{\partial\phi\,\partial r} + \frac{\cos^2\phi\cos\theta}{r^2\sin\theta}\frac{\partial}{\partial\theta}$$
$$+ \frac{\cos^2\phi}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2} - \frac{\sin\phi\cos\phi}{r^2\sin^2\theta}\frac{\partial}{\partial\phi}$$

$$\frac{\partial}{\partial z}\frac{\partial}{\partial z} = \cos^2\theta\frac{\partial^2}{\partial r^2} - \frac{\sin\theta\cos\theta}{r}\frac{\partial^2}{\partial r\,\partial\theta} + \frac{\sin\theta\cos\theta}{r^2}\frac{\partial}{\partial\theta} - \frac{\sin\theta\cos\theta}{r}\frac{\partial^2}{\partial r\,\partial\theta}$$
$$+ \frac{\sin^2\theta}{r}\frac{\partial}{\partial r} + \frac{\sin^2\theta}{r^2}\frac{\partial^2}{\partial\theta^2} + \frac{\sin\theta\cos\theta}{r^2}\frac{\partial}{\partial\theta}$$

Adding the second derivatives,

$$\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} + \frac{\cos\theta}{r^2\sin\theta}\frac{\partial}{\partial\theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$$

or, as it usually is expressed,

$$\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$$