In macromolecular simulation it is often necessary to compute the gradient of internal energy with respect to the Cartesian coordinates (this is necessary, for example, in minimization and molecular dynamics). Most force fields define energy as a function of internal degrees of freedom – that is, distances, angles and dihedral angles between atoms. The functional forms of the energy terms are usually quite simple and their derivatives are trivial. Thus, the most important component is computing partial derivatives of the internal degrees of freedom (i.e. distances, angles and dihedral angles). This can be a bit awkward, especially for angles, because internal coordinates and Cartesian coordinates are related by non-remarkable linear algebraic operations. Here I demonstrate the mathematical formulae, and their derivations, involved in computing these derivatives.

Distance

The distance between points $p_1 = (x_1, y_1, z_1)$ and $p_2 = (x_2, y_2, z_2)$ is $D = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2}$. The derivative of this distance with respect to say x_1 (all coordinates are symmetrical here, so all three derivatives will have the same form), is $\partial D/\partial x_1 = \frac{1}{2\sqrt{(x_1-x_2)^2+(y_1-y_2)^2+(z_1-z_2)^2}} \cdot 2(x_1 - x_2) = \frac{(x_1-x_2)}{\sqrt{(x_1-x_2)^2+(y_1-y_2)^2+(z_1-z_2)^2}}$. Obviously, there is a problem when the two atoms are exactly at the same point because both the numerator and the denominator become zero. Even though this is certainly a case to avoid in actual atomic structures, the code should still not quit with an error or produce incorrect derivatives if this happens. It easy to show that if $y_1 = y_2$ and $z_1 = z_2$, then the limit of the derivative above as $x_1 \to x_2$ is ± 1, where the sign depends on whether the approach is from the positive direction ($x_1 > x_2$) or the negative direction ($x_1 < x_2$). In other words, all partial derivatives at $\vec{r} = (0,0,0)$ are ± 1 (and it makes sense that if two atoms coincide, then the change in each coordinate is also the change in distance to within a sign, since distance is always positive), so this can be handled as a special case in the code. In the code, if x_1 is really exactly the same as x_2 (to within machine precision), we just have to choose a sign in some arbitrary way (e.g. choose the plus sign).

Angle

Suppose we want to find the angle between two vectors: $\vec{r_1} = (a_1, b_1, c_1)$ and $\vec{r_2} = (a_2, b_2, c_2)$. This can be computed as the arccosine of the normalized dot product between the two vectors, or $A = cos^{-1}\left(\frac{a_1a_2+b_1b_2+c_1c_2}{\sqrt{a_1^2+b_1^2+c_1^2}\sqrt{a_2^2+b_2^2+c_2^2}}\right)$. Taking the derivative of this, say with respect to a_1, we get $\frac{\partial A}{\partial a_1} = -\frac{1}{\sqrt{1-d^2}}\left[a_2 \cdot \sqrt{a_1^2 + b_1^2 + c_1^2}\sqrt{a_2^2 + b_2^2 + c_2^2} - (a_1a_2 + b_1b_2 + c_1c_2) \cdot \frac{\sqrt{a_2^2+b_2^2+c_2^2}}{\sqrt{a_1^2+b_1^2+c_1^2}} \cdot a_1\right] \cdot \frac{1}{(a_1^2+b_1^2+c_1^2)(a_2^2+b_2^2+c_2^2)}$ (for shortness, I used d for the argument of the arccosine). It is not hard to see that when the two vectors are collinear (their normalized dot product is 1), this derivative too will have a numerical problem because both the numerator and the denominator will be zero. The entire set of derivatives is:

$$\frac{\partial A}{\partial a_1} = -\frac{1}{\sqrt{1-d^2}}\left[a_2L_1L_2 - p\frac{L_2}{L_1}a_1\right] \cdot \frac{1}{L_1^2L_2^2}$$

$$\frac{\partial A}{\partial a_2} = -\frac{1}{\sqrt{1-d^2}}\left[a_1L_1L_2 - p\frac{L_1}{L_2}a_2\right] \cdot \frac{1}{L_1^2L_2^2}$$

$$\frac{\partial A}{\partial b_1} = -\frac{1}{\sqrt{1-d^2}}\left[b_2 L_1 L_2 - p\frac{L_2}{L_1} b_1\right]\cdot\frac{1}{L_1^2 L_2^2}$$

$$\frac{\partial A}{\partial b_2} = -\frac{1}{\sqrt{1-d^2}}\left[b_1 L_1 L_2 - p\frac{L_1}{L_2} b_2\right]\cdot\frac{1}{L_1^2 L_2^2}$$

$$\frac{\partial A}{\partial c_1} = -\frac{1}{\sqrt{1-d^2}}\left[c_2 L_1 L_2 - p\frac{L_2}{L_1} c_1\right]\cdot\frac{1}{L_1^2 L_2^2}$$

$$\frac{\partial A}{\partial c_2} = -\frac{1}{\sqrt{1-d^2}}\left[c_1 L_1 L_2 - p\frac{L_1}{L_2} c_2\right]\cdot\frac{1}{L_1^2 L_2^2}$$

where for shortness I defined the following quantities: $L_1 = \sqrt{a_1^2 + b_1^2 + c_1^2}$, $L_2 = \sqrt{a_2^2 + b_2^2 + c_2^2}$, $p = a_1 a_2 + b_1 b_2 + c_1 c_2$, and $d = \frac{p}{L_1 L_2}$. Now, supposed that the angle is defined by three points $p_1 = (x_1, y_1, z_1)$, $p_2 = (x_2, y_2, z_2)$, and $p_3 = (x_3, y_3, z_3)$, instead of two vectors, and it is necessary to find the derivative of the angle with respect to the coordinates of the points. In that case, we note that the vectors above relate to the three points as $\vec{r_1} = (a_1 = x_1 - x_2;\ b_1 = y_1 - y_2;\ c_1 = z_1 - z_2)$ and $\vec{r_2} = (a_2 = x_3 - x_2;\ b_2 = y_3 - y_2;\ c_2 = z_3 - z_2)$. Therefore, the angle becomes: $A = cos^{-1}\left(\frac{(x_1-x_2)(x_3-x_2)+(y_1-y_2)(y_3-y_2)+(z_1-z_2)(z_3-z_2)}{\sqrt{(x_1-x_2)^2+(y_1-y_2)^2+(z_1-z_2)^2}\sqrt{(x_3-x_2)^2+(y_3-y_2)^2+(z_3-z_2)^2}}\right)$, and its derivatives with respect to the coordinates of the three points:

$$\frac{\partial A}{\partial x_1} = -\frac{1}{\sqrt{1-d^2}}\left[(x_3 - x_2)L_1 L_2 - p\frac{L_2}{L_1}(x_1 - x_2)\right]\cdot\frac{1}{L_1^2 L_2^2}$$
$$\frac{\partial A}{\partial y_1} = -\frac{1}{\sqrt{1-d^2}}\left[(y_3 - y_2)L_1 L_2 - p\frac{L_2}{L_1}(y_1 - y_2)\right]\cdot\frac{1}{L_1^2 L_2^2}$$
$$\frac{\partial A}{\partial z_1} = -\frac{1}{\sqrt{1-d^2}}\left[(z_3 - z_2)L_1 L_2 - p\frac{L_2}{L_1}(z_1 - z_2)\right]\cdot\frac{1}{L_1^2 L_2^2}$$
$$\frac{\partial A}{\partial x_3} = -\frac{1}{\sqrt{1-d^2}}\left[(x_1 - x_2)L_1 L_2 - p\frac{L_1}{L_2}(x_3 - x_2)\right]\cdot\frac{1}{L_1^2 L_2^2}$$
$$\frac{\partial A}{\partial y_3} = -\frac{1}{\sqrt{1-d^2}}\left[(y_1 - y_2)L_1 L_2 - p\frac{L_1}{L_2}(y_3 - y_2)\right]\cdot\frac{1}{L_1^2 L_2^2}$$
$$\frac{\partial A}{\partial z_3} = -\frac{1}{\sqrt{1-d^2}}\left[(z_1 - z_2)L_1 L_2 - p\frac{L_1}{L_2}(z_3 - z_2)\right]\cdot\frac{1}{L_1^2 L_2^2}$$
$$\frac{\partial A}{\partial x_2} = -\frac{1}{\sqrt{1-d^2}}\left[(2x_2 - x_1 - x_3)L_1 L_2 + p\left\{\frac{L_2}{L_1}(x_1 - x_2) + \frac{L_1}{L_2}(x_3 - x_2)\right\}\right]\cdot\frac{1}{L_1^2 L_2^2}$$
$$\frac{\partial A}{\partial x_2} = -\frac{1}{\sqrt{1-d^2}}\left[(2x_2 - x_1 - x_3)L_1 L_2 + p\left\{\frac{L_2}{L_1}(x_1 - x_2) + \frac{L_1}{L_2}(x_3 - x_2)\right\}\right]\cdot\frac{1}{L_1^2 L_2^2}$$
$$\frac{\partial A}{\partial z_2} = -\frac{1}{\sqrt{1-d^2}}\left[(2z_2 - z_1 - z_3)L_1 L_2 + p\left\{\frac{L_2}{L_1}(z_1 - z_2) + \frac{L_1}{L_2}(z_3 - z_2)\right\}\right]\cdot\frac{1}{L_1^2 L_2^2}$$

where L_1, L_2, p and d are defined as before, except now they will be written in terms of the coordinates of the points. Note that the derivates with respect to the coordinates of the central point are merely the negative sum of the corresponding derivatives with respect to the coordinates of terminal points, which makes perfect geometric sense. Here again we have a singularity issue – when the angle is 0 or 180 (that is $d^2 = 1$), both the numerator and the denominator of the derivatives go to zero, making it impossible to determine the derivatives with the formulae above. The derivative itself must exist, however, for geometric reasons and we can always compute it numerically at any point. Before, with distance, we took the limit of the derivative as the singularity point is approached. Here, we can do the same, but that turns out to be pretty hairy. Instead, we will apply a simple geometric argument akin to the argument regarding distance that the differential of coordinate is also the differential of distance when distance is zero. Lets look at the case where the angle is nearly 0. Then, the angle is the length of the arc connecting the ends of unit vectors along $\vec{r_1}$ and $\vec{r_2}$, which is also approximately the distance between the ends of these unit vectors (and this becomes exact when the angle approaches zero). Given that the angle is zero, if one coordinate of point p_1 or p_3 changes (say it is p_1) by some δ, then the position of the end point of $\vec{r_1}$ changes by the same δ, this translates into a change in this coordinate of the end of one of the unit vector $\frac{\vec{r_1}}{|\vec{r_1}|}$ by an amount $\frac{\delta}{|\vec{r_1}|}$, and the component of this latter change that is orthogonal to the direction of $\vec{r_1}$ is also the change in distance between p_1 and p_3 (to within a sign, since distance is always positive), and also the change in arc length and hence angle. The amount of change of each coordinate that is orthogonal to $\vec{r_1}$ and $\vec{r_2}$ is determined by the angle β, which is π/2 minus the angle between the axis corresponding to the coordinate and $\vec{r_1}$ (or $\vec{r_2}$, which is the same). Thus, for the x-coordinate, $\beta_x = \frac{\pi}{2} - angle(\vec{X}, \vec{r_1}) = \frac{\pi}{2} - arccos\left(\frac{[1,0,0]\cdot\vec{r_1}}{|\vec{r_1}|}\right) = \frac{\pi}{2} - arccos\left(\frac{r_1^x}{|\vec{r_1}|}\right)$, where r_1^x is the x-component of $\vec{r_1}$. The same can be done for y- and z-coordinates. The cosine of the appropriate β, divided by the magnitude of the vector, is then the component of that coordinate's delta that is orthogonal to the vectors. Thus, for the coordinates of points p_1 and p_3, when the angle is very close to zero, the derivatives of the angle can be written as:

$$\frac{\partial A}{\partial x_1} = \pm\frac{\cos(\beta_x)}{|\vec{r_2}|} = \pm\frac{1}{|\vec{r_2}|}\cos\left(\frac{\pi}{2} - arccos\left(\frac{r_2^x}{|\vec{r_2}|}\right)\right) = \pm\frac{1}{|\vec{r_2}|}\sin\left(arccos\left(\frac{r_2^x}{|\vec{r_2}|}\right)\right)$$

$$\frac{\partial A}{\partial y_1} = \pm\frac{\cos(\beta_y)}{|\vec{r_2}|} = \pm\frac{1}{|\vec{r_2}|}\cos\left(\frac{\pi}{2} - arccos\left(\frac{r_2^y}{|\vec{r_2}|}\right)\right) = \pm\frac{1}{|\vec{r_2}|}\sin\left(arccos\left(\frac{r_2^y}{|\vec{r_2}|}\right)\right)$$

$$\frac{\partial A}{\partial z_1} = \pm\frac{\cos(\beta_z)}{|\vec{r_2}|} = \pm\frac{1}{|\vec{r_2}|}\cos\left(\frac{\pi}{2} - arccos\left(\frac{r_2^z}{|\vec{r_2}|}\right)\right) = \pm\frac{1}{|\vec{r_2}|}\sin\left(arccos\left(\frac{r_2^z}{|\vec{r_2}|}\right)\right)$$

$$\frac{\partial A}{\partial x_3} = \pm\frac{\cos(\beta_x)}{|\vec{r_1}|} = \pm\frac{1}{|\vec{r_1}|}\cos\left(\frac{\pi}{2} - arccos\left(\frac{r_1^x}{|\vec{r_1}|}\right)\right) = \mp\frac{1}{|\vec{r_1}|}\sin\left(arccos\left(\frac{r_1^x}{|\vec{r_1}|}\right)\right)$$

$$\frac{\partial A}{\partial y_3} = \pm\frac{\cos(\beta_y)}{|\vec{r_1}|} = \pm\frac{1}{|\vec{r_1}|}\cos\left(\frac{\pi}{2} - arccos\left(\frac{r_1^y}{|\vec{r_1}|}\right)\right) = \mp\frac{1}{|\vec{r_1}|}\sin\left(arccos\left(\frac{r_1^y}{|\vec{r_1}|}\right)\right)$$

$$\frac{\partial A}{\partial z_3} = \pm\frac{\cos(\beta_z)}{|\vec{r_1}|} = \pm\frac{1}{|\vec{r_1}|}\cos\left(\frac{\pi}{2} - arccos\left(\frac{r_1^z}{|\vec{r_1}|}\right)\right) = \mp\frac{1}{|\vec{r_1}|}\sin\left(arccos\left(\frac{r_1^z}{|\vec{r_1}|}\right)\right)$$

The sign, once again, depends on whether the approach to the singularity is from the positive or the negative direction. The meaning of the positive direction here is that the direction of $\vec{X}$, or whichever coordinate we are looking at, is co-directional with $\vec{r_2} - \vec{r_1}$ or opposite to it (i.e. whether the dot product of $\vec{X}$ and $\vec{r_2} - \vec{r_1}$ is positive or negative, respectively), corresponding to positive and negative directions, respectively, and corresponding to a + or a – in the formulae above, respectively. Obviously, when $\vec{r_2}$ and $\vec{r_1}$ are perfectly the same (within machine precision) and so $\vec{r_2} - \vec{r_1}$ is zero, the derivative from left and from right will have different signs (because the angle is decreasing in both directions), so we just have to choose one of them, by convention, in the code (e.g. choose the plus sign). For the middle point p_2, as before, the derivative should be the minus sum of the corresponding derivatives for p_1 and

p_3. This is because moving p_2 by a small amount in some direction is geometrically equivalent in terms of the angle produced to moving p_1 and p_3 each by the same small amount in the opposite direction. Thus:

$$\frac{\partial A}{\partial x_2} = -\frac{\partial A}{\partial x_1} - \frac{\partial A}{\partial x_3};\ \frac{\partial A}{\partial y_2} = -\frac{\partial A}{\partial y_1} - \frac{\partial A}{\partial y_3};\ \frac{\partial A}{\partial z_2} = -\frac{\partial A}{\partial z_1} - \frac{\partial A}{\partial z_3}$$

For the case where the angle is close to π all of the derivatives will be exactly the negative of those above. This can be shown by saying that in that case the angle is $\pi - \varepsilon$, where ε is a very small angle, and so the derivative of this angle will be minus the derivative of this small angle, which is what we did above.

Dihedral angle

The dihedral angle is merely an angle between two planes, or the angle between the normals to the two planes. Suppose we want to find the dihedral angle defined by points $\overrightarrow{P_1} = (x_1, y_1, z_1)$, $\overrightarrow{P_2} = (x_2, y_2, z_2)$, $\overrightarrow{P_3} = (x_3, y_3, z_3)$, and $\overrightarrow{P_4} = (x_4, y_4, z_4)$. This will be the angle between the normals to surfaces $P_1P_2P_3$ and $P_4P_3P_2$, which are formed by the cross products $\overrightarrow{P_1P_2} \times \overrightarrow{P_3P_2}$ and $\overrightarrow{P_4P_3} \times \overrightarrow{P_3P_2}$. Thus, the two normals are:

$$\overrightarrow{N_1} = [(y_1 - y_2)(z_3 - z_2) - (z_1 - z_2)(y_3 - y_2);\ (z_1 - z_2)(x_3 - x_2) - (x_1 - x_2)(z_3 - z_2);\ (x_1 - x_2)(y_3 - y_2) - (y_1 - y_2)(x_3 - x_2)]$$

$$\overrightarrow{N_2} = [(y_4 - y_3)(z_3 - z_2) - (z_4 - z_3)(y_3 - y_2);\ (z_4 - z_3)(x_3 - x_2) - (x_4 - x_3)(z_3 - z_2);\ (x_4 - x_3)(y_3 - y_2) - (y_4 - y_3)(x_3 - x_2)]$$

Therefore, we can treat the dihedral case as just an angle defined by three points $\left[\overrightarrow{N_1}, \overrightarrow{(0,0,0)}, \overrightarrow{N_2}\right]$, reducing the problem to the previous case. Except that there are two issues to deal with. One is that dihedrals have sign (i.e., handedness), whereas we defined angle above as an arccosine, so only over the range $[0, \pi]$. The second is that to get the gradient of the dihedral with respect to the coordinates of its defining points, we still have to apply the chain rule to the gradient of the above angle, which would be with respect to the coordinates of $\overrightarrow{N_1}$ and $\overrightarrow{N_2}$.

We can define the sign based on which side of the plane $\left[\overrightarrow{P_1}, \overrightarrow{P_2}, \overrightarrow{P_3}\right]$ point $\overrightarrow{P_4}$ maps onto. To do so, we can simply compute the sign of the dot product between the normal to the plane $\left[\overrightarrow{P_1}, \overrightarrow{P_2}, \overrightarrow{P_3}\right]$ and the vector $\overrightarrow{P_3P_4}$. So, we can say that $\sigma = \text{sign}\left(\left(\overrightarrow{P_1P_2} \times \overrightarrow{P_3P_2}\right) \cdot \overrightarrow{P_3P_4}\right) = -\text{sign}\left(\left(\overrightarrow{P_1P_2} \times \overrightarrow{P_3P_2}\right) \cdot \overrightarrow{P_4P_3}\right)$. Thus, we can express the dihedral as $D = \sigma \cdot A\left(\overrightarrow{N_1}, \overrightarrow{(0,0,0)}, \overrightarrow{N_2}\right) = \sigma \cdot A_0\left(\overrightarrow{N_1}, \overrightarrow{N_2}\right)$, where function A_0 is defined to be the same as A, except that it assumes the middle point to be at the origin (A_0 is defined purely so that the arguments reflect only just the independent variables and no constants).

To compute the partial derivative of D with respect some coordinate of one of the original four points, lets call it κ, we would apply the chain rule for multiple variables:

$$\frac{\partial D}{\partial \kappa} = \sigma \cdot \left(\frac{\partial A_0}{\partial N_1^x}\frac{\partial N_1^x}{\partial \kappa} + \frac{\partial A_0}{\partial N_1^y}\frac{\partial N_1^y}{\partial \kappa} + \frac{\partial A_0}{\partial N_1^z}\frac{\partial N_1^z}{\partial \kappa} + \frac{\partial A_0}{\partial N_2^x}\frac{\partial N_2^x}{\partial \kappa} + \frac{\partial A_0}{\partial N_2^y}\frac{\partial N_2^y}{\partial \kappa} + \frac{\partial A_0}{\partial N_2^z}\frac{\partial N_2^z}{\partial \kappa}\right)$$

Here is a table of all the needed derivatives with respect to all possible κ (the latter are across the top):

	x_1	y_1	z_1	x_2	y_2	z_2	x_3	y_3	z_3	x_4	y_4	z_4
N_1^x	0	$z_3 - z_2$	$y_2 - y_3$	0	$z_1 - z_3$	$y_3 - y_1$	0	$z_2 - z_1$	$y_1 - y_2$	0	0	0
N_1^y	$z_2 - z_3$	0	$x_3 - x_2$	$z_3 - z_1$	0	$x_1 - x_3$	$z_1 - z_2$	0	$x_2 - x_1$	0	0	0
N_1^z	$y_3 - y_2$	$x_2 - x_3$	0	$y_1 - y_3$	$x_3 - x_1$	0	$y_2 - y_1$	$x_1 - x_2$	0	0	0	0
N_2^x	0	0	0	0	$z_4 - z_3$	$y_3 - y_4$	0	$z_2 - z_4$	$y_4 - y_2$	0	$z_3 - z_2$	$y_2 - y_3$
N_2^y	0	0	0	$z_3 - z_4$	0	$x_4 - x_3$	$z_4 - z_2$	0	$x_2 - x_4$	$z_2 - z_3$	0	$x_3 - x_2$
N_2^z	0	0	0	$y_4 - y_3$	$x_3 - x_4$	0	$y_2 - y_4$	$x_4 - x_2$	0	$y_3 - y_2$	$x_2 - x_3$	0

Each independent variable is in one column and only the non-zero entries in each column (and the corresponding terms in the chain-rule equation above) end up being involved. Note that for the first three and the last three independent variables (i.e., the coordinates of the first and the fourth points) there are only two terms involved, whereas there are four terms for the middle four variables (the middle two points). So, we can now compute all the necessary derivatives:

$$\frac{\partial D}{\partial x_1} = \sigma \cdot \left(\frac{\partial A_0}{\partial N_1^y}(z_2 - z_3) + \frac{\partial A_0}{\partial N_1^z}(y_3 - y_2) \right)$$

$$\frac{\partial D}{\partial y_1} = \sigma \cdot \left(\frac{\partial A_0}{\partial N_1^x}(z_3 - z_2) + \frac{\partial A_0}{\partial N_1^z}(x_2 - x_3) \right)$$

$$\frac{\partial D}{\partial z_1} = \sigma \cdot \left(\frac{\partial A_0}{\partial N_1^x}(y_2 - y_3) + \frac{\partial A_0}{\partial N_1^y}(x_3 - x_2) \right)$$

$$\frac{\partial D}{\partial x_2} = \sigma \cdot \left(\frac{\partial A_0}{\partial N_1^y}(z_3 - z_1) + \frac{\partial A_0}{\partial N_1^z}(y_1 - y_3) + \frac{\partial A_0}{\partial N_2^y}(z_3 - z_4) + \frac{\partial A_0}{\partial N_2^z}(y_4 - y_3) \right)$$

$$\frac{\partial D}{\partial y_2} = \sigma \cdot \left(\frac{\partial A_0}{\partial N_1^x}(z_1 - z_3) + \frac{\partial A_0}{\partial N_1^z}(x_3 - x_1) + \frac{\partial A_0}{\partial N_2^x}(z_4 - z_3) + \frac{\partial A_0}{\partial N_2^z}(x_3 - x_4) \right)$$

$$\frac{\partial D}{\partial z_2} = \sigma \cdot \left(\frac{\partial A_0}{\partial N_1^x}(y_3 - y_1) + \frac{\partial A_0}{\partial N_1^y}(x_1 - x_3) + \frac{\partial A_0}{\partial N_2^x}(y_3 - y_4) + \frac{\partial A_0}{\partial N_2^y}(x_4 - x_3) \right)$$

$$\frac{\partial D}{\partial x_3} = \sigma \cdot \left(\frac{\partial A_0}{\partial N_1^y}(z_1 - z_2) + \frac{\partial A_0}{\partial N_1^z}(y_2 - y_1) + \frac{\partial A_0}{\partial N_2^y}(z_4 - z_2) + \frac{\partial A_0}{\partial N_2^z}(y_2 - y_4) \right)$$

$$\frac{\partial D}{\partial y_3} = \sigma \cdot \left(\frac{\partial A_0}{\partial N_1^x}(z_2 - z_1) + \frac{\partial A_0}{\partial N_1^z}(x_1 - x_2) + \frac{\partial A_0}{\partial N_2^x}(z_2 - z_4) + \frac{\partial A_0}{\partial N_2^z}(x_4 - x_2) \right)$$

$$\frac{\partial D}{\partial z_3} = \sigma \cdot \left(\frac{\partial A_0}{\partial N_1^x}(y_1 - y_2) + \frac{\partial A_0}{\partial N_1^y}(x_2 - x_1) + \frac{\partial A_0}{\partial N_2^x}(y_4 - y_2) + \frac{\partial A_0}{\partial N_2^y}(x_2 - x_4) \right)$$

$$\frac{\partial D}{\partial x_4} = \sigma \cdot \left(\frac{\partial A_0}{\partial N_2^y}(z_2 - z_3) + \frac{\partial A_0}{\partial N_2^z}(y_3 - y_2) \right)$$

$$\frac{\partial D}{\partial y_4} = \sigma \cdot \left(\frac{\partial A_0}{\partial N_2^x}(z_3 - z_2) + \frac{\partial A_0}{\partial N_2^z}(x_2 - x_3) \right)$$

$$\frac{\partial D}{\partial z_4} = \sigma \cdot \left(\frac{\partial A_0}{\partial N_2^x}(y_2 - y_3) + \frac{\partial A_0}{\partial N_2^y}(x_3 - x_2) \right)$$