Hessian terms

The idea now is that for every energy term i will add the Hessian terms that will be needed.

I already have the Hessian of the area i also need to add later the hessian of the Dihedral angle

$$u = p_2 - p_1 \quad v = p_3 - p_1 \quad w = p_4 - p_1 \tag{1}$$

The idea now is to write the terms of the Hessian here

We consider also that

$$\begin{align} g &= \det(u, v, w)||u|| \tag{2} \\ h &= \langle u \times w, v \times u \rangle \tag{3} \\ f &= \arctan 2(g, h) \tag{4} \\ r &= g^2 + h^2 \tag{5} \end{align}$$

Now we calculate the derivatives

$$\begin{align} f_u &= f_h h_u + f_g g_u \tag{6} \\ &= \frac{1}{r}\left(-gu^T([w]_x[v]_x + [v]_x[w]_x) + h(||u||(v \times w)^T + det(u, v, w)\frac{u^T}{||u||})\right) \tag{7} \end{align}$$

$$\begin{align} f_v &= f_h h_v + f_g g_v \tag{8} \\ &= \frac{1}{r}\left(-gw^T[u]_x^2 + h||u||(w \times u)^T\right) \tag{9} \end{align}$$

$$\begin{align} f_w &= f_h h_w + f_g g_w \tag{10} \\ &= \frac{1}{r}\left(-gv^T[u]_x^2 + h||u||(u \times v)^T\right) \tag{11} \end{align}$$

Now that we have differentiated with all the variables we can say how is the gradient for every point.

$$f_{p_1} = -f_u - f_v - f_w \quad f_{p_2} = f_u \quad f_{p_3} = f_v \quad f_{p_4} = f_w \tag{12}$$

And those are the terms of the gradient of f. Lets remember that f is the dihedral angle.

Now we will do the Hessian of the dihedral angle

Considering

$$l = v \times w \quad B = [w]_x[v]_x + [v]_x[w]_x \quad \alpha = \det(u, v, w) \tag{13}$$

$$f_{p_2p_2} = \frac{g^2 - h^2}{r^2}\left[||u||(Bu \otimes l + l \otimes Bu) + \frac{\alpha}{||u||}(Bu \otimes u + u \otimes Bu)\right] \tag{14}$$

$$+ \frac{2gh}{r^2}\Big[Bu \otimes Bu - ||u||^2 l \otimes l\Big] + \frac{1}{r^2}\left(-2gh\alpha + \frac{hr}{||u||}\right)(l \otimes u + u \otimes l) \tag{15}$$

$$- \left(\frac{2gh\alpha^2}{r^2||u||^2} - \frac{h\alpha r}{r^2||u||^3}\right)(u \otimes u) - \frac{g}{r}B + \frac{h\alpha}{||u||r}\mathcal{I} \tag{16}$$

This one is the ugliest actually, the other ones are nicer

First $f_{p_3p_3}$ courtesy of Christian, assuming this

$$a = w \times u \quad b = u \times (u \times w) = a \times u \tag{17}$$

$$f_{p_3p_3} = \frac{2gh}{r^2}\Big(b \otimes b - ||u||^2 a \otimes a\Big) + \frac{||u||(g^2 - h^2)}{r^2}(a \otimes b + b \otimes a) \tag{18}$$

The next one is $f_{p_4p_4}$. In this case we consider

$$d = u \times v \quad k = u \times (u \times v) = u \times d \tag{19}$$

And the terms are

$$f_{p_4p_4} = \frac{2gh}{r^2}\Big(k \otimes k - ||u||^2 d \otimes d\Big) + \frac{||u||(g^2 - h^2)}{r^2}(d \otimes k + k \otimes d) \tag{20}$$

And those are the diagonal terms, now we will do the off diagonals.

We will define some things also

$$C = (-2[w]_x[u]_x + [u]_x[w]_x) \tag{21}$$

So the next term is $f_{p_2p_3}$

$$f_{p_2p_3} = \frac{g^2-h^2}{r^2}\left[-||u||Cv \otimes a + ||u||l \otimes b + \frac{\alpha}{||u||}u \otimes b\right] \tag{22}$$

$$+ \frac{2gh}{r^2}\left[Cv \otimes b + ||u||^2 l \otimes a + \alpha u \otimes a\right] - \frac{g}{r}C \tag{23}$$

And now we have $f_{p_2p_4}$

We define a matrix as

$$D = -2[v]_x[u]_x + [u]_x[v]_x \tag{24}$$

$$f_{p_2p_4} = \frac{g^2-h^2}{r^2}\left[||u||Dw \otimes d + ||i||l \otimes (u \times d) + \frac{\alpha}{||u||}u \otimes (u \times d)\right] \tag{25}$$

$$+ \frac{2gh}{r^2}[Dw \otimes (u \times d) - ||u||l \otimes d - \alpha u \otimes d] - \frac{g}{r}D + \frac{h}{r}\left(||u||[v]_x + \frac{1}{||u||}u \otimes d\right) \tag{26}$$

And now we have $f_{p_4p_3}$

$$f_{p_4p_3} = \frac{g^2-h^2}{r^2}[-||u||k \otimes a + ||u||d \otimes b] \tag{27}$$

$$+ \frac{2gh}{r^2}\left[||u||^2 d \otimes a + k \otimes b\right] - \frac{g}{r}[u]_x^2 + \frac{h||u||}{r}[u]_x \tag{28}$$

Now we can do the rest of the terms

$$f_{p_1p_1} = (-f_{p_2} - f_{p_3} - f_{p_4})_{p1} \tag{29}$$

$$= f_{p_2p_2} + f_{p_2p_3} + f_{p_2p_4} + f_{p_3p_2} + f_{p_3p_3} + f_{p_3p_4} + f_{p_4p_2} + f_{p_4p_3} + f_{p_4p_4} \tag{30}$$

Lets do the rest

$$f_{p_1p_2} = (-f_{p_2} - f_{p_3} - f_{p_4})_{p2} \tag{31}$$

$$= -f_{p_2p_2} - f_{p_3p_2} - f_{p_4p_2} \tag{32}$$

$$f_{p_1p_3} = (-f_{p_2} - f_{p_3} - f_{p_4})_{p3} \tag{33}$$

$$= -f_{p_2p_3} - f_{p_3p_3} - f_{p_4p_3} \tag{34}$$

$$f_{p_1 p_4} = (-f_{p_2} - f_{p_3} - f_{p_4})_{p4} \tag{35}$$

$$= -f_{p_2 p_4} - f_{p_3 p_4} - f_{p_4 p_4} \tag{36}$$

Ok, now lets write the rest of the hessians. To take a small break i will write the Hessian of an edge

Let $u = p_2 - p_1$

$$l(u) = ||u|| \tag{37}$$

From out previous experience we know

$$l_{p1} = -l_u \quad l_{p2} = l_u \tag{38}$$

Thefore the term of the gradient is

$$l_u = \frac{u^T}{||u||} \quad l_{p1} = -\frac{u^T}{||u||} \quad l_{p2} = \frac{u^T}{||u||} \tag{39}$$

And now the for the Hessian we now

$$l_{uu} = l_{p_1 p_1} = l + p_2 p_2 = \frac{1}{||u||}\left(\mathcal{I} - \frac{u \otimes u}{||u||^2}\right) \tag{40}$$

Now for the off diagonal terms, hmm... in this case i think they just have a minus sign at the front.

$$l_{p_1 p_2} = -(l_u)_u = -\frac{1}{||u||}\left(\mathcal{I} - \frac{u \otimes u}{||u||^2}\right) \tag{41}$$

Now we can do the Hessian of the area, we will use the same notation as before, so we have

$$u = p_2 - p_1 \quad v = p_3 - p_1 \quad u_{p_1} = -id \quad u_{p_2} = id \quad v_{p_1} = -id \quad v_{p_3} = id \tag{42}$$

Let $z = u \times v \quad z_v = [u]_\times \quad z_u = -[v]_\times$

Considering $A = ||z||$ (This is actually twice the area but we just need to remember to divide the results by two at the the end)

$$A_z = \frac{z^T}{||z||} \tag{43}$$

$$A_u - A_z z_u = -\frac{1}{||z||} z^T [v]_\times = \frac{1}{||z||}([v]_\times z)^T \tag{44}$$

$$= \frac{1}{||z||}(v \times z)^T \tag{45}$$

$$A_v = A_z z_v = \frac{1}{||z||} z^T [u]_\times = \frac{1}{||z||}([u]_\times^T z)^T \tag{46}$$

$$= -\frac{1}{||z||}(u \times z)^T \tag{47}$$

Now that we have the partial derivatives we can write the gradient of the area

$$A_{p_1} = A_u u_{p_1} + A_v v_{p_1} \tag{48}$$

$$= -A_u - A_v \tag{49}$$

$$= -\frac{1}{||z||}((u - v) \times z)^T \tag{50}$$

$$= -\frac{1}{|z||}((p_2 - p_3) \times z)^T \tag{51}$$

$$A_{p_2} = \frac{1}{||z|vert}((p_3 - p_1) \times z)^T \tag{52}$$

$$A_{p_3} = \frac{1}{||z||}((p_1 - p_2) \times z)^T \tag{53}$$

Perfect, now that we have the first derivatives its time to write down the second derivatives.

Thanks to Christian we got this

$$A_{p_1p_1} = \frac{1}{||z||}\left(\frac{-((u-v)\times z)\cdot((u-v)\times z)^T}{||z||^2} - [u-v]_\times^2\right) \tag{54}$$

$$A_{p_2p_2} = -\frac{1}{||z||}\left(\frac{1}{||z|^2}((p_3-p_1)\times z)((p_3-p_1)\times z) + [p_3-p_1]_\times^2\right) \tag{55}$$

$$A_{p_3p_3} = -\frac{1}{||z||}\left(\frac{1}{||z|^2}((p_1-p_2)\times z)((p_1-p_2)\times z) + [p_1-p_2]_\times^2\right) \tag{56}$$

$$A_{p_2p_3} = \frac{1}{||z||}\left([p_3-p_1]_\times(id - \frac{zz}{||z||^2})[p_2-p_1]_\times - [z]_\times\right) \tag{57}$$

$$A_{p_3p_1} = \frac{1}{||z||}\left([p_1-p_2]_\times(id - \frac{zz}{||z||^2})[p_3-p_2]_\times - [z]_\times\right) \tag{58}$$

$$A_{p_1p_2} = \frac{1}{||z||}\left([p_2-p_3]_\times(id - \frac{zz}{||z||^2})[p_1-p_3]_\times - [z]_\times\right) \tag{59}$$

I think those are all the terms that i need for now. I still need to add the interactions with the Bead but lets do that later because we require considering dot products :(

Assembling the Hessian

Ok so this is the part where we dialog the structure of the code to get my Hessian.

According to Christian I should create functions that take a vector and return the Block hessians.

For the area hessian i should have

- `gradient`$_area([p1p2, p3]) This function takes a 9-dimensional vector with the coordinates of the three vertices and ret$ $vector that contains the gradient of the area with respect to each of the vertices.$

This functions should be implemented simply because there will be a bigger function that will ensamble the rest of the info.