Documentation for MCell Grid Utilities

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The surface grid utilities can be found in the files `grid_util.h` and `grid_util.c`

1 Theory

Consider a triangle with vertices A, B, C. We will orient the $\hat{u}$ axis along the line from A to B and the $\hat{v}$ axis perpendicular according to the right-hand rule. Thus, A is at $(0, 0)$, B is at $u_B \cdot \hat{u}$ and C is at $u_C \cdot \hat{u} + v_C \cdot \hat{v}$. Suppose that we subdivide this triangle into n equal pieces along each edge, creating n^2 subtriangles (see Figure 1).

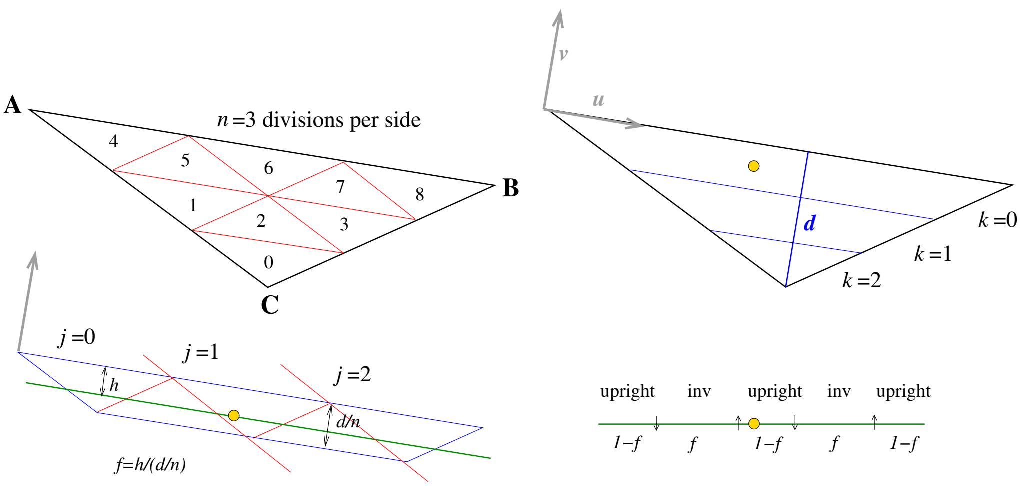

Figure 1: A barycentrically subdivided triangle (top left) consists of n^2 subtriangles (red) identical to the original save for flipping. These can be numbered in n strips as demonstrated. If you hit a spot on the original triangle (gold dot, top right), you can quickly find which row it is in, and then the portion of the way through the row (bottom left). Finally, the line can be segmented into original-orientation and inverted-orientation segments and the position within that line noted (bottom right).

1.1 u, v coordinates to barycentric index

Any point P in the triangle ABC will have a $\hat{v}$ coordinate between 0 and v_C. Barycentric subdivision will split this into n equal strips and thus P will be in the $k = \left\lfloor \frac{n \cdot v_P}{v_C} \right\rfloor$'th strip (counting from 0 to $n-1$). Furthermore, one can find that P is a fraction $f = \frac{v_P - k \cdot v_C / n}{v_C / n} = \frac{n \cdot v_P}{v_C} - k$ of the way to the next strip (see Figure 1). At P, the triangle stretches from $u_0 = u_C \frac{v_P}{v_C}$ to $u_1 = u_B + (u_C - u_B) \frac{v_P}{v_C}$ along the u axis, which we can map to $2k+1$ regions as shown in Figure 1. We thus can find j between 0 and k using $j = \left\lfloor \frac{u_P - u_0}{u_1 - u_0} \right\rfloor$ and then find if the remainder $\frac{u_P - u_0}{u_1 - u_0} - j$ is less than $1 - f$. If so, let $i = 0$ (upright triangle), otherwise set $i = 1$ (inverted triangle). Then we have the $2j + i$'th triangle in the k'th strip, and there are $(n - k - 1)^2$ triangles in higher-numbered strips so the barycentric index is $b = (n - k - 1)^2 + 2j + i$.

1.2 Barycentric index to u, v coordinates

We can write the barycentric index b as $b = \left\lfloor \sqrt{b} \right\rfloor^2 + r$ and $r = 2\left\lfloor \frac{r}{2} \right\rfloor + \left(r - 2\left\lfloor \frac{r}{2} \right\rfloor\right)$. Using the results of section 1.1, we thus have $k = n - \left\lfloor \sqrt{b} \right\rfloor - 1$, $j = \left\lfloor \frac{r}{2} \right\rfloor = \left\lfloor \frac{b - \left\lfloor \sqrt{b} \right\rfloor^2}{2} \right\rfloor$, and $i = r - 2j$. We then have two cases. If $i = 0$, the triangle is upright. The A-corner starts at $\left(\frac{j}{n} u_B + \frac{k}{n} u_C\right) \hat{u} + \frac{k}{n} v_C \cdot \hat{v}$, and the center of the large triangle is at $\left(\frac{u_B + u_C}{3}\right) \hat{u} + \frac{v_C}{3} \hat{v}$. Since the small triangle is n times smaller along each axis, the centroid of the triangle is thus at $\left(\frac{3j+1}{3n} u_B + \frac{3k+1}{3n} u_C\right) \hat{u} + \frac{3k+1}{3n} v_C \cdot \hat{v}$. If $i = 1$, the triangle is inverted and the A-corner is on the $k+1$'st line, so our corner is at $\left(\frac{j}{n} u_B + \frac{k+1}{n} u_C\right) \hat{u} + \frac{k+1}{n} v_C \cdot \hat{v}$, and since the triangle is inverted, the centroid is flipped in the $\hat{v}$ direction, and thus is offset by $\left(\frac{u_B + u_C}{3n}\right) \hat{u} - \frac{v_C}{3n} \hat{v}$ from the corner. Thus the centroid is at $\left(\frac{3j+1}{3n} u_B + \frac{3k+4}{3n} u_C\right) \hat{u} + \frac{3k+2}{3n} v_C \cdot \hat{v}$. These two results for different i can be rewritten as follows: $\left(\frac{3j+1}{3n} u_B + \frac{3k+1+3i}{3n} u_C\right) \hat{u} + \frac{3k+1+i}{3n} v_C \cdot \hat{v}$.

2 Implementation

There are three grid utility functions (so far). Please see the `grid_util.c` file for explanations.