Volume 76 (2020)

Supporting information for article:

Isotopy classes for 3-periodic net embeddings

Stephen Power, Igor Baburin and Davide Proserpio
Supporting Information

The proof of Theorem 9.5.

Proof. Let $\mathcal{M}$ be model net with adjacency depth 1 and a single vertex quotient graph. We show that $\mathcal{M}$ is equivalent to one of the 19 model nets by an elementary affine transformation.

The case $m = 3$. In all cases it is clear that $\mathcal{M}$ is equivalent to $\mathcal{M}_{\text{pcu}}$.

The case $m = 4$. We consider 4 subcases:

(i) Assume that 3 of the edges of $F_e$ are axial edges. Then $\mathcal{M}$ is obtained from $\mathcal{M}_{\text{pcu}}$ by the addition of an additional edge to the motif. If this is a facial edge then, by rotation and translation $\mathcal{M}$ is equivalent to $\mathcal{M}_{\text{pcu}}^f$, the model net for the word $a_xa_ya_zf_x$. If the extra edge is a diagonal edge then $\mathcal{M}$ is equivalent to $\mathcal{M}_{\text{pcu}}^d$.

(ii) Assume that exactly 2 of the 4 edges of $F_e$ are axial edges. We may these are $a_x, a_y$ and we may also assume that neither of the remaining 2 edges is in the $xy$-plane since in this case there would be a triple of coplanar edges in $F_e$ and $\mathcal{M}$ would be equivalent to $\mathcal{M}_{\text{pcu}}^f$. Suppose first that there is no diagonal edge and so $\mathcal{M}$ is of type $a_xa_yw$ with $w$ one of $f_xf_y, f_xg_y, g_xf_y, g_xg_y$. These nets are pairwise equivalent by rotation about the $z$-axis and translation. By an elementary affine transformation they are thus all equivalent to $\mathcal{M}_{\text{pcu}}^d$.

Assume on the other hand that only 1 of the 2 extra edges is a facial edge. Translating and rotating we may assume that this edge is $f_x$. Also we may assume a noncoplanarity position of the diagonal edge with respect to $f_x$ and $a_x$, as in Figure 1, since otherwise there is an oriented affine equivalence with the model net for $\text{hex}$.

![Figure 1. Some motifs of type $aafd$.](image-url)
The resulting 2 model nets, \( M_1 \) and \( M_2 \) are equivalent by a rotation about the line through the centre of the cube in the \( x \)-axis direction. Thus \( M_1 \) and \( M_2 \) are equivalent to the model net \( M_{aad}^0 \) for the word \( a_xa_yg_zd_1 \).

(iii) Assume that exactly 1 of the 4 edges of \( F_e \) is an axial edge, which we may assume lies in the \( x \)-axis. If the 3 remaining edges are the \( f \)-edges that are incident to the origin, then the transformation of \( M \) by the map \((x, y, z) \rightarrow (x - z, y, z)\) has type \( aaad \) and so is equivalent to \( M_{pcu}^d \). If the 3 remaining \( f \) edges are not of this form then they are either coplanar (and, as before, \( M \) is equivalent to \( M_{pcu}^f \)) or only 1 of these 3 edges is incident to the origin, as in Figure 2. In these cases \( M \) is equivalent to a model net with 2 axial edges and so the previous arguments suffice.

![Figure 2. A motif with 3 non coplanar facial edges.](image)

Thus we may assume that the defining word for \( M \) is of type \( affd, afgd \) or \( aggd \). Moreover by rotational and translational equivalence we may assume that the possible types are \( a_xffd_1, a_xfgd_1 \) or \( a_xggd_1 \). If all four edges are incident to the origin then \( M \) is equivalent by an elementary affine transformation to a model net with 2 axial edges and so there are no new cases to consider. Also if 3 edges are incident to the origin then once again the net is equivalent to the net for \( \text{hex} \), and so it remains to consider the cases \( a_xg_zg_1d_1, a_xg_zg_1d_1 \) and \( a_xg_yg_zd_1 \) indicated in Figure 3.

Note that the first and third nets are the nets \( M_{aad}^{gg} \) and \( M_{ad}^{gg} \) in the list of model nets. That these nets are not isomorphic follows from their topological density counts. The second net has a rotation about the diagonal which is a mirror image of the first net and so is equivalent to it by elementary transformations.

(iv) Finally, for the case \( m = 4 \), we assume that there are no axial edges. By rotational symmetry there are 4 cases which, under the convention are uniquely specified by the words \( fffd, ffgd, fggd \) and \( gggd \). The last of these corresponds to a disconnected net, as we have seen in the previous section, the first gives an alternative model net for \( \text{ic} \) (as we have remarked prior to the proof), and the other 2 nets, for \( ffgd \) and \( fggd \), are easily seen to be affinely equivalent to a model net with 1 axial edge.

**The case** \( m = 5 \). It is straightforward to see that if \( M \) has 3 axial edges and 2 face edges then it is equivalent to the model net \( M_{pcu}^{ff} \) for \( \text{bct} \). Also, type \( aaaaaf \) is equivalent
to this type. On the other hand, type $aaagd$ has hxl-multiplicity equal to 1, rather than 2, and so is in a new equivalence class, also with no edge penetrations. In fact this model net has topology $ile$.

Consider next the model nets with 2 axial edges and no diagonal edges. These also have no penetrating edges and are of hxl-multiplicity 1 or 2. Moreover it is straightforward to show that each is equivalent by elementary affine transformations to a model net with 3 axial edges and so they equivalent to the model nets for $bct$ and $ile$ respectively. The same is true for the 9 nets of type $aawd$ where $w$ is a word in 2 facial edges which is not of type $gg$.

Thus, in the case of 2 axial edges it remains to consider the types $a_xa_ywd_1$ with $w = g_xg_y,g_xg_z$ and $g_yg_z$ each of which has a penetrating edge of type $4^2$. The first two of these are model nets in the list and give new and distinct affine equivalence classes in view of their penetration type and differing hxl($\mathcal{N}$) count. The third net, for the word $a_xa_yg_yg_zd_1$ is a mirror image of the first net and so is orientedly affinely equivalent to it.

It remains to consider the case of 1 axial edge, $a_x$, together with $d_1$ and 3 facial edges. If there are 2 edges of type $f_x,f_y$ or $f_z$ then there is an elementary equivalence with a model net with 2 axial edges. The same applies if there is a single such edge. For an explicit example consider $a_xf_xg_yg_zd_1$. The image of this net under the transformation $(x,y,z) \rightarrow (x,y-z,z)$ gives a depth 1 net with 2 axial edges. The transformation of motifs is indicated in Figure 4.
Finally the model net for $a_x g_y g_z d_1$ appears in the listing and gives a new affine class with penetration type $3^2$.

**The case** $m = 6$. We first assume that there is no diagonal edge in the motif for $\mathcal{M}$ and therefore no edge penetration of type $4^2$ or $3^2$. There are 2 distinguished model nets in the list for this case, one with the 3 facial edges of type $f$ (a net with topology $\text{ild}$) and one where the 3 facial edges are of type $g$ (a net with topology $\text{fcu}$). Two other choices of facial edges are possible (up to rotation) and these are readily seen to be equivalent to the $\text{ild}$ and $\text{fcu}$ nets.

We may now assume that there exists a diagonal edge in the standardised form of the edge word defining $\mathcal{M}$. If there are 3 axial edges then there are 3 possibilities, namely types $aaa f f d$, $aaa f g d$, $aaaggd$. The first 2 cases are not new, since the transformation $(x, y, z) \to (x, y - z, z)$ give motifs without a diagonal edge, while the model net for $aaaggd$ appears in the list, with penetration type $4^2$ and $\text{hxl}(\mathcal{M}) = 2$.

We may now assume that $\mathcal{M}$ has a standardised word $a_x a_y w d_1$ where $w$ is a word in 3 facial edges. For $w$ of $fff$ type there are 3 cases, namely $f_x f_y g_z$, $f_x g_y f_z$ and $g_x f_y f_z$, each of which transforms by an elementary transformation (respectively, $x \to x - z, y \to y - z$ and $x \to x - z$) to a case with 3 axial edges. For $w$ of type $fgg$ there are 3 cases, namely $f_x g_y g_z$, $g_x f_y g_z$ and $g_x g_y f_z$. The first and second of these are not new, since the transformations $y \to y - z$ and $x \to x - z$, respectively, lead to an equivalence with $\mathcal{M}^{ggd}_{\text{pcu}}$, while the third case is the model net $\mathcal{M}^{ggf}_{add}$.

Finally, for $w$ of type $ggg$ we have the model net $\mathcal{M}^{ggg}_{add}$.

**The case** $m = 7$. There are 4 cases of standardised edge word of the form $a a a w d$ with $w$ of type $fff$, $ffg$, $fgg$ or $ggg$. The model net for $a_x a_y a_z f_x f_y f_z d$ is obtained from the model net for $a_x a_y a_z f_x f_y g_z d$ by the transformation $y \to y - z$ followed by a rotation. Thus there is a maximum of 3 equivalence classes with representative model nets $\mathcal{M}^{fff}_{\text{pcu}}, \mathcal{M}^{ggf}_{\text{pcu}}, \mathcal{M}^{ggg}_{\text{pcu}}$. Since these are distinguished by their edge penetration type the proof is complete.  \qed