Growth functions of periodic space tessellations

B. Naskręcki[1,2], J. Malinowski[3], Z. Dauter[4], M. Jaskólski[5,6]

[1]Faculty of Mathematics and Computer Science, Adam Mickiewicz University, Poznań, [2]Poland, Mathematical Institute, Polish Academy of Sciences, Warszawa, Poland, [3]Faculty of Pure and Applied Mathematics, Wrocław University of Science and Technology, Wrocław, Poland, [4]Macromolecular Crystallography Laboratory, NCI, Argonne National Laboratory, Argonne, USA, [5]Department of Crystallography, Faculty of Chemistry, Adam Mickiewicz University, Poznań, Poland, and [6]Institute of Bioorganic Chemistry, Polish Academy of Sciences, Poznań, Poland)

jakub.malinowski@pwr.edu.pl

From mathematical point of view crystal structure can be treated as tessellation of the Euclidean space. In the presented project we investigate relative growth functions of periodic tessellation which are restricted by either topological paths or parallelogram frames. We call the latter type of function “crystallographic” growth functions. The main reason for studying the growth functions is the expectation that such data might be enough to encode tessellation’s space group or even the whole information about tessellation.

Crystallographic growth functions are sensitive to the choice of the anchor point of the frames. We can divide the space (the set of all potential anchor points) into regions within which the growth functions are identical. We call visualisation of this division an ”orphic diagram”. Example orphic diagram is shown in Fig. 1.

As part of the project Julia and SageMath packages dedicated to the growth functions have been created. The packages find growth functions and create orphic diagrams. The results returned by the packages are exact. Numerical errors are eliminated by using symbolic calculations.

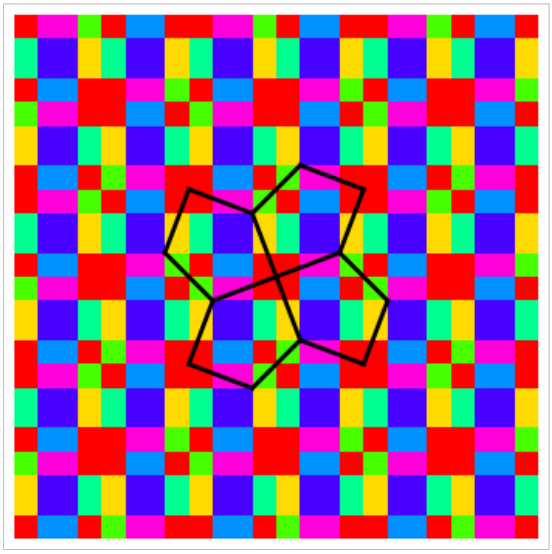

Figure 1. Simplified orphic diagram for Cairo pentagonal tilling

[1] B. Naskrecki, J. Malinowski, Z. Dauter and M. Jaskolski, Growth functions of periodic space tessellations., Acta Crystallographica Section A., 2025, 81(1):64-81

[2] B. Naskrecki, Z. Dauter and M. Jaskolski, A topological proof of the modified Euler characteristic based on the orbifold concept., Acta Crystallographica Section A., 2021, 77(4):317–326