Interactive 2D Periodic Graphs

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Abstract

We present an educational web app for interactively drawing and editing 2D periodic graphs. The user defines the unit cell and the finite set of vertex and edge representatives, from which a sufficiently large fragment of the periodic graph is created for the visualization. The periodic graph can also be modified by applying several transformations, including isometries and relaxations of the unit cell. A finite representation of the infinite periodic graph can be saved in an external file as a quotient graph with Z^2-marked edges. Its geometry is recorded using fractional (crystallographic) coordinates. The facial structure of non-crossing periodic graphs can be revealed by the user interactively selecting face representatives. An accompanying video demonstrates the functionality of the web application.

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1 Introduction

Motivated by applications in crystallography and materials science [4], periodic graphs have been studied intensely in recent years in the context of rigidity of bar-and-joint frameworks [1, 2, 3, 5]. They also appear in computational topology as the universal cover of geodesic toroidal drawings [6, 7]. We present an educational web app to create, edit, visualize and generate finite descriptions of 2D geometric periodic graphs (Fig. 1).

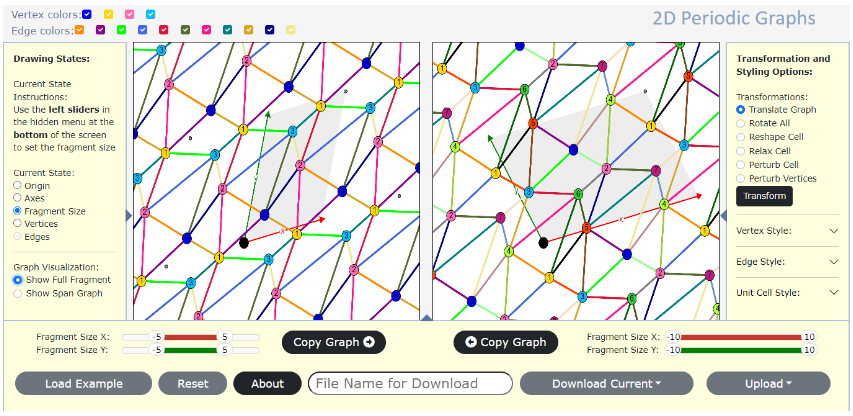

Figure 1 The drawing canvas (left) and transformation canvas (right) display a fragment of the same (infinite) crystal up to isometries and relaxation of periodicity. Translation, rotation and relaxation transformations have been applied on the left graph to obtain the one on the right. Vertices or edges of the same color belong to the same orbit. The shaded parallelogram represents the unit cell, shown together with its origin and generating vectors.

Informally, a *periodic graph* is an infinite graph with a translationally-repeating finite pattern of vertices and edges. In 2D, periodic graphs can be generated from two independent translation vectors that induce a *unit cell* and a finite number of vertices and edges, called *representatives*. The infinite periodic graph is partitioned into a finite set of vertex and edge orbits, which receive distinct *colors*. We describe an interactive web app, available at `http://linkage.cs.umass.edu/pergraph/`, which can facilitate the study and visualization of various properties of periodic graphs.

The web application has two canvases, one for drawing and one for applying transformations. There are three hidden menus (left, right, and bottom) that can be opened by hovering over them. Fig. 1 shows all three of them. An accompanying video, accessed through the *Video* option in the bottom menu or directly at `http://linkage.cs.umass.edu/pergraph/about/`, briefly demonstrates the functionality of the app and includes additional information and features not discussed in this abstract.

2 Crystals and their representations

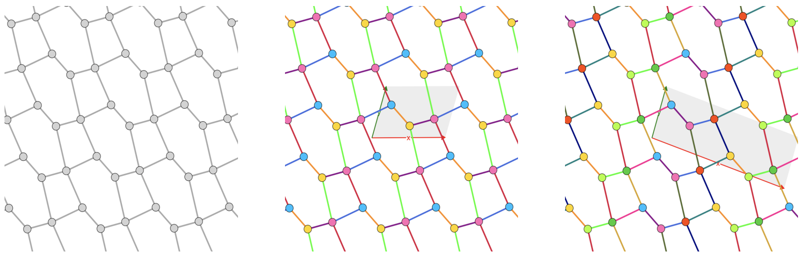

Figure 2 (Left) A 2D crystal. (Middle and right) Two of its possible periodic graphs. The highlighted unit cells represent the periodicity groups, and vertices or edges in the same orbit get identical colors.

Crystals and Periodic Graphs. A *2D crystal* (Fig. 2, left) is an infinite graph which (a) is locally finite (each vertex is incident to finitely many edges) and (b) is subject to the action of *some* periodicity group. Condition (b) actually implies the existence of infinitely many periodicity groups acting on the same crystal: if we fix the group action, we obtain a specific *periodic graph* [1]. Fig. 2 (middle and right) shows two distinct periodic graphs obtained from the same crystal. We specify a periodicity group by its generators (two vectors, the red x-axis and the green y-axis inducing the gray *unit cell*) and use colors to indicate the group action: similarly colored vertices (resp. edges) belong to the same *orbit*.

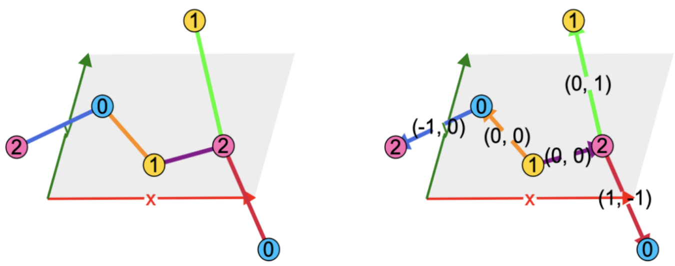

Figure 3 An undirected span-graph (left) and the (directed) shift-span-graph (right) of the periodic graph from Fig. 2 (middle). The pair of integers on a directed edge representative indicates the shift of the head-vertex; the tail of the edge representative is always chosen to be in the unit cell.

Quotient and shift-quotient graphs. To each periodic graph we associate a *quotient-graph*, whose vertices V (resp. edges E) correspond to orbits (colors) of vertices (resp. edges) in the original periodic graph. It is, in general, a multi-graph. The information in the quotient graph (V, E) is insufficient for reconstructing the periodic graph [1, 2] and must be supplemented by Z^2-markings (called *shifts*) on directed versions of the quotient graph edges. This type of *marked directed multi-graph* associated to a periodic graph is called a *shift-quotient-graph*. The *shift* is a pair $(i, j) \in Z^2$ of integers. A *shift-edge* is a *pair* of an edge $(u, v) \in V$ in the quotient graph and a shift (i, j). It stands for an edge representative whose tail is the representative of vertex orbit u and whose head is a translation (that goes i-times in the direction of the x-axis and j-times in the direction of the y-axis) of the vertex representative v. The x and y-axes are the generators of the periodicity lattice. The shift-quotient-graph is a complete finite description of a periodic graph and is used in the `.sqf` file format for exporting the graphs produced by our web app.

Span and shift-span graphs. For visualization purposes we use a geometric version of (shift)-quotient-graphs called *(shift)-span-graphs*. A *span-graph* (Fig. 3 (left)) is a subgraph of the geometric periodic graph. It contains all the edge-representatives selected as follows. We first choose vertex representatives to be in the unit cell. An edge representative for an orbit of edges is chosen so that one of its endpoints (the tail) is in the unit cell; the second endpoint (the head) may be either inside or outside of the unit cell. In a span-graph each edge representative appears exactly once (each with its unique edge color). However, several geometric points with the same color (representing vertices from the same vertex orbit) may be present among the edge representative endpoints. The span-graph is thus a *simple* (no multi-edges) colored geometric graph. A *shift-span-graph* (Fig. 3 (right)) orients the edges of the span graph and marks them with shifts such that the *tail* is always inside the unit cell. In short: *the (shift)-quotient graph is obtained by identifying vertices of the same color in the (shift)-span-graph.*

Fractional coordinates. The geometry of the crystal vertices can be expressed using *fractional coordinates* of the vertex representatives relative to the unit cell axes. We use them in the geometric version of the shift-quotient-graphs recorded in the external (file) representation of the graphs produced by our web app.

Crystal fragment. Given the two generators of the unit cell (x- and y-axes), a shift-quotient graph and fractional coordinates for the vertices, we can reconstruct a *fragment* of the infinite periodic graph. We need a position for the *origin* to build the *unit cell* from the two axes. From this information we compute the Cartesian coordinates of the vertex representatives from the fractional ones. Finally, we use two integer-intervals *(windows)* indicating the range of translations of the unit cell in the x and y-directions necessary to build a fragment. The windows can be selected by the user so that the fragment covers the canvas.

Finite descriptions of crystals. Periodicity groups already provide infinitely many ways to describe the same geometric crystal. Furthermore, each periodicity group may be described in infinitely many ways by different choices of generators (unit cells). Two choices of unit cells lead to the same quotient graph as long as they have the same index. If the unit cell is relaxed, then the number of vertices and edges in the quotient graph is scaled by an integer factor. In Fig. 2, the graph on the right is a relaxation of index 2 of the periodic graph in the middle and thus the number of vertices and edges of its quotient-graph are doubled.

Transformations of crystals and periodic graphs. Geometric crystals can be translated or rotated, or be represented by different periodicity groups. Each periodicity group can be represented by different unit cells, resulting in the same number of vertices in the unit cell. All these different representations may result in different fractional coordinates of the vertex representatives. Finally, we may choose different orientations for the edge representatives and obtain different shifts. *Our web app software captures this multitude of different ways of obtaining finite periodic graph representations of the same infinite crystal.*

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