Computing fundamental domains of crystallographic groups

With connections to topological interlocking

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GAPDays Summer 2024

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Lemma

Let $E(n)$ be the set of all isometries of a dimension $n \in \mathbb{N}$. Then $E(n)$ is a group with the composition of homomorphisms as the group operation.

Proposition ([4, Exa. 1.1, Prop. 1.6])

There is an isometry

$$E(n) \cong O(n) \ltimes \mathbb{R}^n.$$

We denote with φ_o the orthogonal part of φ and with φ_t the vector/translation part of φ.

Then the group operation of $\varphi, \psi \in E(n)$ is as follows:

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$$(\varphi_o, \varphi_t) \circ (\psi_o, \psi_t) := (\underbrace{\varphi_o \circ \psi_o}_{\substack{\text{op. in } O(n) \\ \text{i.e. comp. of maps}}}, \psi_t^{\varphi_o} + \varphi_t),$$

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$$\mathbb{R}^n \times (O(n) \ltimes \mathbb{R}^n) \to \mathbb{R}^n : (v, (\varphi_o, \varphi_t)) \mapsto v^{(\varphi_o, \varphi_t)} = v^{\varphi_o} + \varphi_t.$$

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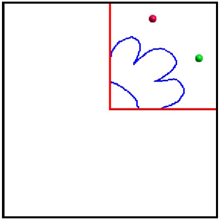
(i) $\bigcup_{\gamma\in\Gamma} F^{\langle\gamma\rangle} = \mathbb{R}^n$,

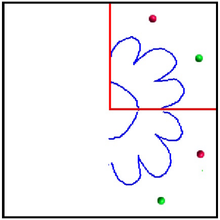
(ii) there is a system of representatives $V \subseteq \mathbb{R}^n$ w.r.t. the partition given by the orbits of Γ acting on $\mathbb{R}^n$ such that

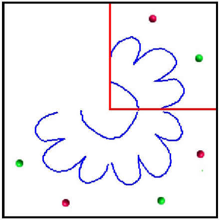
$$F^\circ \subseteq V \subseteq F.$$

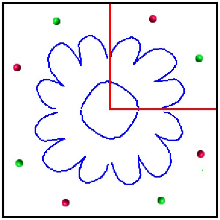
Example

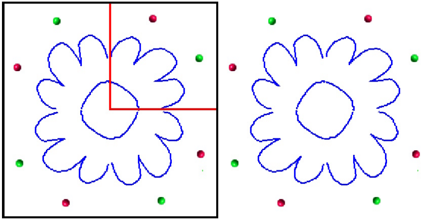
$$p4 := \left\langle \rho := \left(\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \end{pmatrix}^T \right), \right.$$
$$\tau_1 := \left(\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \end{pmatrix}^T \right),$$
$$\left. \tau_2 := \left(\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}^T \right) \right\rangle$$

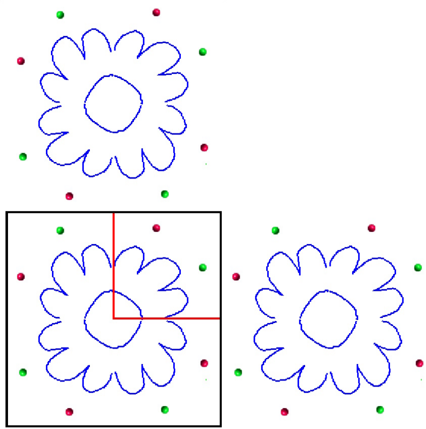


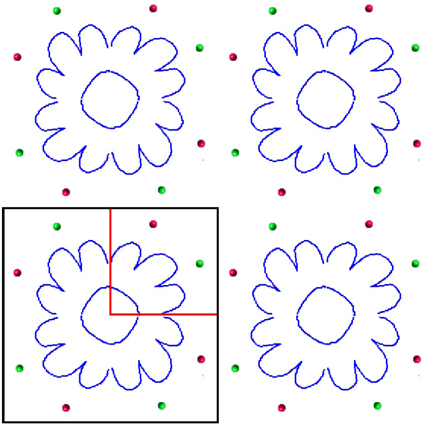


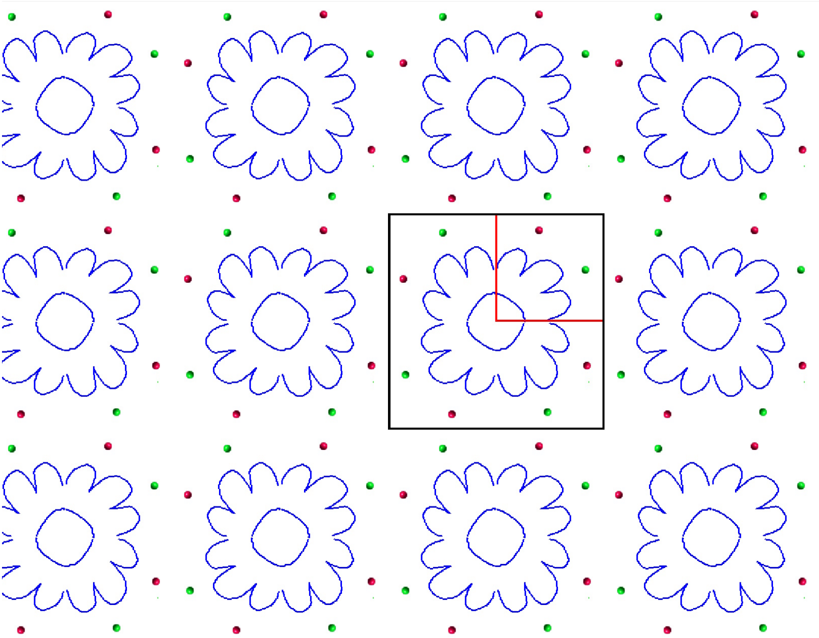












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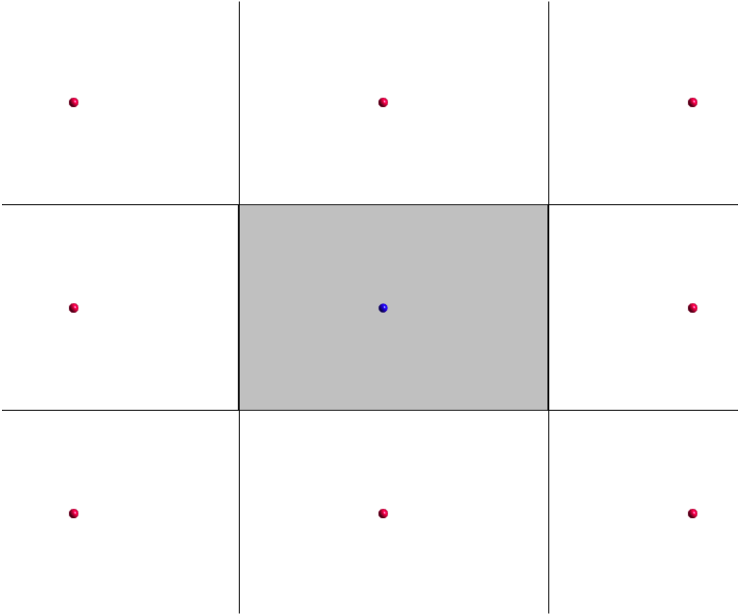
Definition ([3, Def. III.1])

Let $O \subseteq \mathbb{R}^n$ be a discrete set and $u \in O$ be a point. We call

$$D(u, O) = \bigcap_{w \in O, w \neq u} H^+(u, w).$$

the *Dirichlet cell of u*.



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Theorem ([2, Thm. III.11 (ii)])

Let $\Gamma \leq E(n)$ be a crystallographic group and $u \in \mathbb{R}^n$ a point in general position.

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Theorem ([2, Thm. III.11 (ii)])

Let $\Gamma \leq E(n)$ be a crystallographic group and $u \in \mathbb{R}^n$ a point in general position. Then the Dirichlet cell $D(u, u^\Gamma)$ is a fundamental domain for Γ.

Definition ([1, §3, Thm. 7, with remark after])

Let $B \subset \mathbb{R}^n$ be a closed subset. We define the *volume* of B as the Lebesgue measure of B, so $\mathrm{vol}(B) := \lambda(B)$ in the notation of [1].

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Let $B \subset \mathbb{R}^3$ a closed subset, $\varphi \in E(3)$.

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It can be shown that all fundamental domains of crystallographic groups have the same volume.

Remark

For every crystallographic group Γ there is a certain subgroup called the translation subgroup that is denoted by

$$\mathcal{T}(\Gamma) \leq \Gamma.$$

Theorem

Let $\Gamma \leq E(n)$ be a crystallographic group with fundamental domain F and $u \in \mathbb{R}^n$ a point in general position. Then we choose a generating set for Γ and I, K finite index sets, such that

$$\Gamma = \langle \rho_i, \tau_k \mid i \in I, k \in K \rangle,$$

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Then there is an $A \in \mathbb{N}$ such that the Dirichlet cell $D(u, u^\Gamma)$ is the intersection of halfspaces $H^+(u, w)$ for words w of length at most $A + 1$.

Algorithm 3.2: Dirichlet Cell

Data: a crystallographic group $\Gamma = \langle \rho_i, \tau_k \mid i \in I, k \in K \rangle \leq E(n)$ such that $\Gamma = \cup_{i \in I} \rho_i \mathcal{T}(\Gamma)$, a point u in general position w.r.t. Γ and the maximal *length* of words in *gens* to check

Result: *triangularComplex*, a triangular complex that is a fundamental domain.

wordsOfLenghtL $\leftarrow$ all words in the generators *gens* of length at most *length*

for γ *in wordsOfLenghtL* **do**

  Add(elementsInOrbit, u^γ);

end

halfspaces $\leftarrow$ halfspaces $H_{u,v}$ for all $v \in$ *elementsInOrbit*;

fundDom $\leftarrow$ triangular complex given by intersection of *halfspaces*;

return *fundDom*;

Time for some examples

Example

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Next steps

- Implement above in SimplicialSurfaces Package
- Improve algorithm by automatically running until expected volume is reached
- Check if h-vector conversion can be done more efficiently
- Consider numerical effects

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Goal is to deform fundamental domains in such a way, that they continue to be fundamental domains but also fulfill the *topological interlocking property*.

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Definition

A block $B \subseteq \mathbb{R}^3$ is called topologically interlocking, if there is an assembly of it, such that by fixing a subset of the assembly there is no subset of the remaining blocks that can be moved without intersecting any blocks.

Thank you for your attention

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