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Delone lattice studies in $\mathbf{C^3}$, the space of three complex variables

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Abstract

The Delone (Selling) scalars, which are used in unit cell reduction and in lattice type determination, are studied in $\mathbf{C^3}$, the space of 3 complex variables. The 3 complex coordinate planes are composed of the 6 Delone scalars.

Note: In his later publications, Boris Delaunay used the Russian version of his surname, Delone.

1. Introduction

The scalars used by Delaunay (1932) in his formulation of Selling reduction (Selling, 1874) are (in the conventional order) $b \cdot c$, $a \cdot c$, $a \cdot b$, $a \cdot d$, $b \cdot d$, $c \cdot d$, where $d = -a-b-c$.

(As a mnemonic device, observe that the first three terms use α, β, and γ, in that order, and the following terms use a, b, c, in that order.)

Andrews *et al.* (2019b) chose to represent the Selling scalars in the space $\mathbf{S^6}$, $\{s_1$, s_2, s_3, s_4, s_5, $s_6\}$ (defined in the order above), as a way to create a metric space for the measurement of the distance between lattices. They also consider the representation of this space as the space of three complex dimensions, $\mathbf{C^3}$ or $\{c_1$, c_2, $c_3\}$.

In $\mathbf{C^3}$, in terms of the Selling scalars, a vector is defined as $\{(s_1,s_4)$, (s_2,s_5),$(s_3,s_6)\}$, where the real and imaginary parts of each are the "opposite" scalars according to the definition of Delaunay (1932) (see Andrews *et al.* (2019a)). As a mnemonic device, note that the complex components involve (α, a), (β, b), and (γ, c). Additionally, each complex term uses all four 3-space vectors; for example, c_1 is $(b \cdot c,\ a \cdot d)$.

Andrews *et al.* (2019b) considered the matrix representations of the reflections in $\mathbf{C^3}$ (and in $\mathbf{S^6}$). This paper describes the boundary transformations at the edges of the fundamental unit of $\mathbf{C^3}$. In $\mathbf{S^6}$, the fundamental unit is the all negative orthant, which contains only and all of the reduced cells. In $\mathbf{S^6}$ and $\mathbf{C^3}$, the boundaries located where any $\mathbf{S^6}$ scalar (or correspondingly in$\mathbf{C^3}$, the real or imaginary part) equals to zero. The rationale for this work was that it might lend insights into the topology of the space of lattices.

2. Notation

Complex numbers will be represented in Cartesian format (x, y), where x is the real part and y is the imaginary part.

We will represent a vector in $\mathbf{C^3}$ by $\{(x_1, y_1)$, (x_2, y_2), $(x_3, y_3)\}$ as an alternative to $\{(s_1,s_4)$, (s_2,s_5),$(s_2,s_6)\}$.

Next we define the operators in $\mathbf{C^3}$ t hat will be used in the matrix descriptions of the transformations at the boundaries of the fundamental unit.

See Table 1.

Table 1. *The Result column values give the products of each operator as applied to* (x_j, y_j)

Operator	Usage	Result	Name
$\mathfrak{M}_r$	$\mathfrak{M}_r(c_j)$	$(-x_j, -x_j + y_j)$	Minus real
$\mathfrak{M}_i$	$\mathfrak{M}_i(c_j)$	$(x_j - y_j, -y_j)$	Minus imag
$\mathfrak{P}_r$	$\mathfrak{P}_r(c_j)$	(x_j, x_j)	Plus real
$\mathfrak{P}_i$	$\mathfrak{P}_i(c_j)$	(y_j, y_j)	Plus imag
$\Re$	$\Re\ (c_j)$	x_j	Real
$\Im$	$\Im\ (c_j)$	y_j	Imaginary

.

3. Matrices of boundary transformations

For the boundary at s_1: (the real component of c_1).

$$\begin{bmatrix}\mathfrak{M}_r & 0 & 0\\ \mathfrak{P}_r & \mathrm{i}\Re & \Re\\ \mathfrak{P}_r & \mathrm{i}\Im & \Im\end{bmatrix}\begin{bmatrix}\mathfrak{M}_r & 0 & 0\\ \mathfrak{P}_r & \mathrm{i}\Im & \Im\\ \mathfrak{P}_r & \mathrm{i}\Re & \Re\end{bmatrix}\begin{bmatrix}\mathfrak{M}_r & 0 & 0\\ \mathfrak{P}_r & \Re & \mathrm{i}\Re\\ \mathfrak{P}_r & \Im & \mathrm{i}\Im\end{bmatrix}\begin{bmatrix}\mathfrak{M}_r & 0 & 0\\ \mathfrak{P}_r & \Im & \mathrm{i}\Im\\ \mathfrak{P}_r & \Re & \mathrm{i}\Re\end{bmatrix}$$

For the boundary at s_4: (the imaginary component of c_1).

$$\begin{bmatrix}\mathfrak{M}_i & 0 & 0\\ \mathfrak{P}_i & \mathrm{i}\Re & \Re\\ \mathfrak{P}_i & \mathrm{i}\Im & \Im\end{bmatrix}\begin{bmatrix}\mathfrak{M}_i & 0 & 0\\ \mathfrak{P}_i & \mathrm{i}\Im & \Im\\ \mathfrak{P}_i & \mathrm{i}\Re & \Re\end{bmatrix}\begin{bmatrix}\mathfrak{M}_i & 0 & 0\\ \mathfrak{P}_i & \Re & \mathrm{i}\Re\\ \mathfrak{P}_i & \Im & \mathrm{i}\Im\end{bmatrix}\begin{bmatrix}\mathfrak{M}_i & 0 & 0\\ \mathfrak{P}_i & \Im & \mathrm{i}\Im\\ \mathfrak{P}_i & \Re & \mathrm{i}\Re\end{bmatrix}$$

For the boundary at s_2 (the real component of c_2):

$$\begin{bmatrix}\mathrm{i}\Re & \mathfrak{P}_r & \Re\\ 0 & \mathfrak{M}_r & 0\\ \mathrm{i}\Im & \mathfrak{P}_r & \Im\end{bmatrix}\begin{bmatrix}\mathrm{i}\Im & \mathfrak{P}_r & \Im\\ 0 & \mathfrak{M}_r & 0\\ \mathrm{i}\Re & \mathfrak{P}_r & \Re\end{bmatrix}\begin{bmatrix}\Re & \mathfrak{P}_r & \mathrm{i}\Re\\ 0 & \mathfrak{M}_r & 0\\ \Im & \mathfrak{P}_r & \mathrm{i}\Im\end{bmatrix}\begin{bmatrix}\Im & \mathfrak{P}_r & \mathrm{i}\Im\\ 0 & \mathfrak{M}_r & 0\\ \Re & \mathfrak{P}_r & \mathrm{i}\Re\end{bmatrix}$$

For the boundary at s_5: (the imaginary component of c_2).

$$\begin{bmatrix}\mathrm{i}\Re & \mathfrak{P}_i & \Re\\ 0 & \mathfrak{M}_i & 0\\ \mathrm{i}\Im & \mathfrak{P}_i & \Im\end{bmatrix}\begin{bmatrix}\mathrm{i}\Im & \mathfrak{P}_i & \Im\\ 0 & \mathfrak{M}_i & 0\\ \mathrm{i}\Re & \mathfrak{P}_r i & \Re\end{bmatrix}\begin{bmatrix}\Re & \mathfrak{P}_i & \mathrm{i}\Re\\ 0 & \mathfrak{M}_i & 0\\ \Im & \mathfrak{P}_i & \mathrm{i}\Im\end{bmatrix}\begin{bmatrix}\Im & \mathfrak{P}_i & \mathrm{i}\Im\\ 0 & \mathfrak{M}_i & 0\\ \Re & \mathfrak{P}_i & \mathrm{i}\Re\end{bmatrix}$$

For the boundary at s_3 (the real component of c_3):

$$\begin{bmatrix}\mathrm{i}\Re & \Re & \mathfrak{P}_r\\ \mathrm{i}\Im & \Im & \mathfrak{P}_r\\ 0 & 0 & \mathfrak{M}_r\end{bmatrix}\begin{bmatrix}\mathrm{i}\Im & \Im & \mathfrak{P}_r\\ \mathrm{i}\Re & \Re & \mathfrak{P}_r\\ 0 & 0 & \mathfrak{M}_r\end{bmatrix}\begin{bmatrix}\Re & \mathrm{i}\Re & \mathfrak{P}_r\\ \Im & \mathrm{i}\Im & \mathfrak{P}_r\\ 0 & 0 & \mathfrak{M}_r\end{bmatrix}\begin{bmatrix}\Im & \mathrm{i}\Im & \mathfrak{P}_r\\ \Re & \mathrm{i}\Re & \mathfrak{P}_r\\ 0 & 0 & \mathfrak{M}_r\end{bmatrix}$$

For the boundary at s_6 (the imaginary component of c_3):

$$\begin{bmatrix}\mathrm{i}\Re & \Re & \mathfrak{P}_i\\ \mathrm{i}\Im & \Im & \mathfrak{P}_i\\ 0 & 0 & \mathfrak{M}_i\end{bmatrix}\begin{bmatrix}\mathrm{i}\Im & \Im & \mathfrak{P}_i\\ \mathrm{i}\Re & \Re & \mathfrak{P}_i\\ 0 & 0 & \mathfrak{M}_i\end{bmatrix}\begin{bmatrix}\Re & \mathrm{i}\Re & \mathfrak{P}_i\\ \Im & \mathrm{i}\Im & \mathfrak{P}_i\\ 0 & 0 & \mathfrak{M}_i\end{bmatrix}\begin{bmatrix}\Im & \mathrm{i}\Im & \mathfrak{P}_i\\ \Re & \mathrm{i}\Re & \mathfrak{P}_i\\ 0 & 0 & \mathfrak{M}_i\end{bmatrix}$$

4. Basics

The standard representation of the identity operation is

$$\mathbf{c}' = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \mathbf{c}.$$

The identity in $\mathbf{C^3}$ can also be written:

$$\mathbf{c}' = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \Re + \mathrm{i}\Im & 0 \\ 0 & 0 & \Re + \mathrm{i}\Im \end{bmatrix} \mathbf{c}.$$

Delaunay (1932) does not consider the boundary transformations in detail. However, he uses them to define the process of Selling reduction. For example in $\mathbf{S^6}$, he lists the following as one of the possible results for a transformation on s_1: $\{-s_1, -s_1{+}s_2, s_1{+}s_3, s_1{+}s_5, s_1{+}s_4, s_1{+}s_6\}$. The third boundary transform for s_1 implements this operation and interchanges the real part of c_3 and the imaginary part of c_2:

$$\begin{bmatrix} \mathfrak{M}_r & 0 & 0 \\ \mathfrak{P}_r & \Re & \mathrm{i}\Re \\ \mathfrak{P}_r & \Im & \mathrm{i}\Im \end{bmatrix}$$

Considered in $\mathbf{C^3}$, Delone's alternate transformation for the s_1 boundary would exchange the real of c_2 with the imaginary part of c_3. That is the fourth matrix in the list for s_1. The other two transformations for s_1 can be generated from the two we have just displayed by the "exchange operation" (Andrews *et al.*, 2019b) applied to the second and third $\mathbf{C^3}$ coordinates. Delone did not describe the latter two transformation, perhaps because even a single transformation was adequate to implement reduction. He already listed two.

5. Graphical display of projections

The 2-dimensional nature of the three coordinates of $\mathbf{C^3}$ suggests their use for graphical display.

As an example, we use Phospholipase A2 (retrieved from the Protein Data Bank (Bernstein *et al.*, 1977)), which has had several similar or identical structures determined (Le Trong & Stenkamp, 2007). Andrews *et al.* (2019b) found additional cases (see Table 2)

PDB id	Centering	a	b	c	α	β	γ
1DPY	R	57.98	57.98	57.98	92.02	92.02	92.02
1FE5	R	57.98	57.98	57.98	92.02	92.02	92.02
1G0Z	H	80.36	80.36	99.44	90	90	120
1G2X	C	80.95	80.57	57.1	90	90.35	90
1U4J	H	80.36	80.36	99.44	90	90	120
2OSN	R	57.10	57.10	57.10	89.75	89.75	89.75

Table 2. *Phospholipase A2 unit cells*

Below, Figure 1 shows the unit cells as reported (the centering of lattices has not been removed). The following figures show various transformations and embellishments of the reported cells.

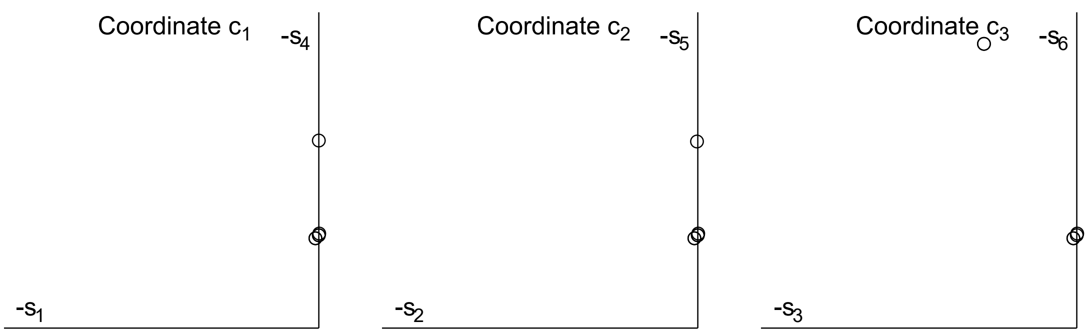

Fig. 1. Phospholipase A2 unit cells as reported.

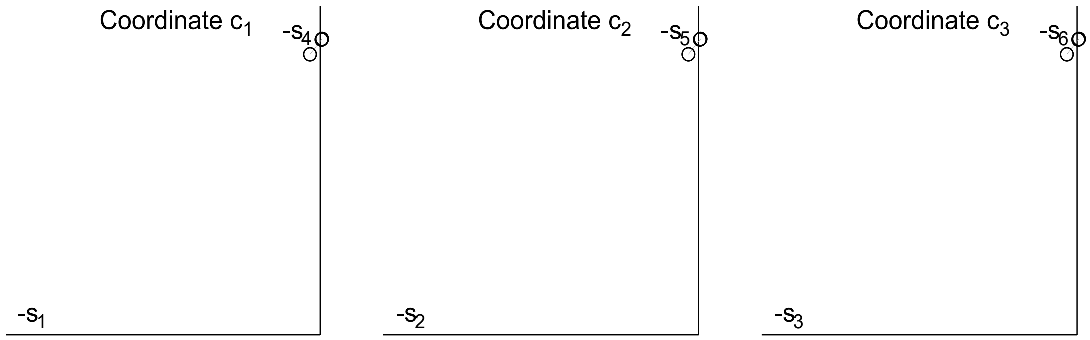

Fig. 2. The unit cells Niggli reduced. The similarity of the 3 projections is indicative of the exact or nearly exact rhombohedral symmetry.

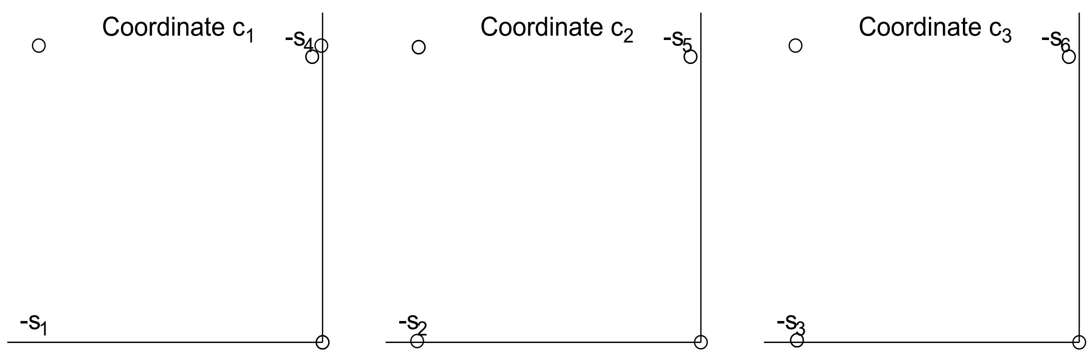

Fig. 3. The unit cells Delone reduced.

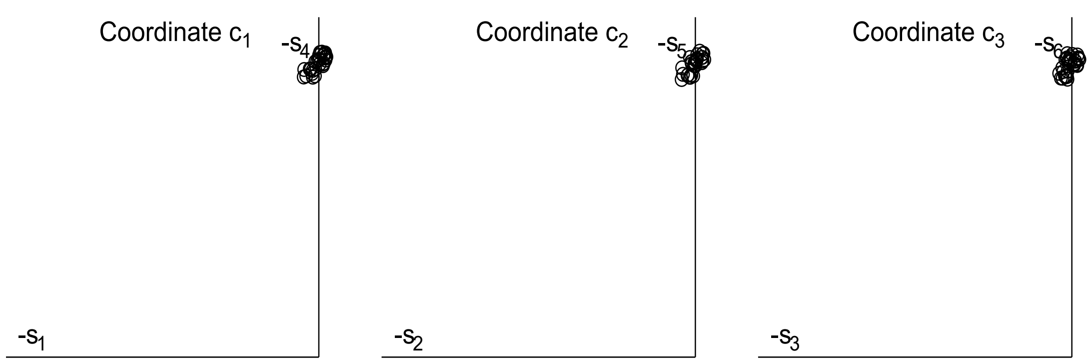

Fig. 4. The unit cells, Niggli and 5 copies were perturbed 2% orthogonally to $\mathbf{S^6}$ vector.

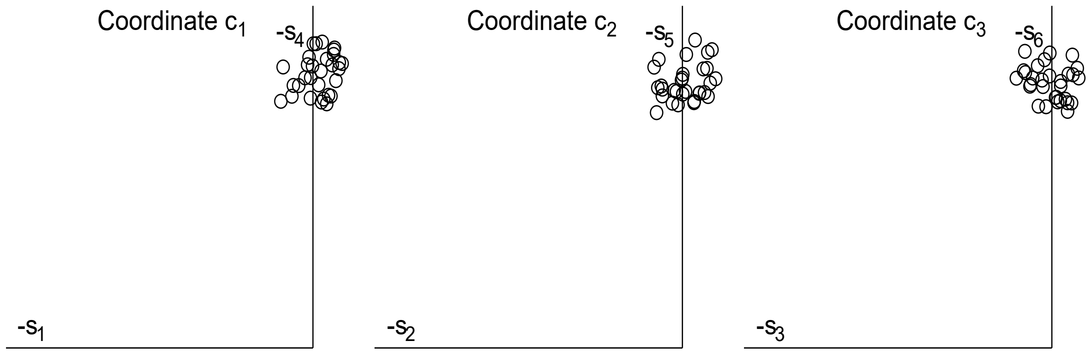

Fig. 5. The unit cells Niggli, and 5 copies were perturbed 10% orthogonally to $\mathbf{S^6}$ vector.

6. Summary

The transformation matrices shown above demonstrate the considerable regularity of Selling reduction, as used by Delaunay (1932), in comparison to Niggli reduction (Niggli, 1928). While all the boundaries of the non-positive orthant of $\mathbf{S^6}$ are essentially the same (and related by reflections), the boundaries formed in Niggli reduction are of multiple types, and the fundamental unit of the space representing Niggli reduced cells ($\mathbf{G^6}$, see Andrews & Bernstein (2014)) is non-convex.

The matrices also display one of the unique properties of $\mathbf{C^3}$, which makes it a useful conceptual representation. For the scalar being transformed, it and its opposite scalar create a unique row in each transformation matrix. These rows contain only the minus operator and zeros, highlighting the unique relationship of that pair of scalars.

Several aspects of $\mathbf{C^3}$ are evident from inspecting the matrices. First, each boundary has four possible transformations that can be applied. Since each of the transformations at boundaries are self-inverse, they are the same transformations that would be used in the process of cell (lattice) reduction. Delaunay (1932) and Delone *et al.* (1975) give only two choices, presumably for simplicity, omitting transformations that use the "exchange" operator (see Andrews *et al.* (2019b)).

7. Availability of code

The C^{++} code for $\mathbf{C^3}$ is available in github.com, in `https://github.com/duck10/LatticeRepLib.git`.

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Synopsis

The space $\mathbf{C^3}$ is explained in more detail than in the original description. Boundary transformations of the fundamental unit are described in detail. A graphical presentation of the basic coordinates is described and illustrated.